ProDy

Protein Dynamics & Sequence Analysis

Interactions Analysis

Release

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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  2024 5kqm_all_sci.pdb
222K Feb 29  2024 addH_5kqm.pdb
3.3M Feb 29  2024 addH_7laf.pdb
4.5M Feb 29  2024 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.getFrequentInteractors()` method:

```
In [18]: interactions.getFrequentInteractors(contacts_min=4)
```

```
@> VAL8P  <---> hb:ASP42P  hp:LEU89P  hp:PHE26P  hb:ARG40P
@> LEU9P  <---> hp:ALA44P  hp:PHE85P  hb:LEU89P  hp:ILE77P  hb:TYR87P
@> CYS12P  <---> hb:ASN15P  hb:SER19P  hb:THR46P  hb:ALA44P
@> ASN15P  <---> hb:HIS72P  hb:ARG75P  hb:CYS12P  hb:SER19P  hb:SER43P
@> ARG18P  <---> hb:ALA22P  hb:ASP92P  sb:ASP92P  hb:ILE127P  sb:ASP129P  hp:VAL141P
@> GLU23P  <---> hb:ARG27P  hb:ARG27P  hb:ARG27P  sb:ARG27P  sb:HIS72P  hb:SER19P
@> VAL25P  <---> hb:LEU29P  hp:LEU29P  hb:ILE21P  hp:TYR142P
@> PHE26P  <---> hp:VAL8P  hb:VAL30P  hp:VAL30P  ps:TRP39P  hp:VAL41P  hb:ALA22P
@> ARG27P  <---> hb:THR31P  hb:GLU23P  hb:GLU23P  hb:GLU23P  sb:GLU23P
@> LYS28P  <---> hb:ASP32P  sb:ASP32P  hb:ALA24P  hp:ILE68P
@> TRP39P  <---> hp:LYS6P  hp:ILE35P  hp:LEU153P  ps:PHE26P  hb:SER36P
@> ARG40P  <---> hb:VAL8P  pc:PHE85P  hb:LYS6P  hb:THR84P  hp:PHE85P
@> ASP42P  <---> hb:PHE10P  hb:ARG75P  sb:ARG75P  hb:VAL8P
@> ALA44P  <---> hb:CYS12P  hp:ARG75P  hp:LEU9P  hb:PHE10P
@> ASP56P  <---> hb:ARG58P  hb:ARG58P  hb:ARG58P  sb:ARG58P  hb:GLN60P  hb:ILE16P
@> ARG58P  <---> hb:CYS62P  hb:ASP56P  hb:ASP56P  hb:ASP56P  sb:ASP56P  hb:TYR131P  hb:TYR131P  hp:H
@> MET63P  <---> hp:ILE21P  hb:ILE68P  hp:ILE68P  hp:ALA24P  hb:GLY59P
@> ARG65P  <---> pc:HIS66P  sb:GLU139P  hb:SER61P  hb:GLU139P
@> HIS66P  <---> ps:TYR142P  pc:ARG65P  hb:GLU139P  sb:GLU139P
@> ARG75P  <---> hb:ALA45P  sb:ASP81P  hb:ASN15P  hb:ASP42P  sb:ASP42P  hp:ALA44P  hb:ASP81P  hb:ASP
@> ILE77P  <---> hp:LEU9P  hp:LYS102P  hb:ALA45P  hp:LEU99P
@> ASP81P  <---> hb:ARG75P  hb:ARG75P  hb:THR78P  hb:PHE85P  sb:ARG75P  hb:THR78P
@> PHE85P  <---> hp:ARG40P  hp:LEU9P  pc:ARG40P  hb:ASP81P
@> ASP86P  <---> hb:SER7P  sb:LYS110P  hb:LYS112P  hb:SER7P
@> ILE88P  <---> hp:VAL11P  hp:PHE82P  hp:ALA111P  hb:GLU114P  hb:LYS112P
```

```
@> LEU89P  <--->  hb:VAL11P  hp:TYR119P  hp:VAL8P  hb:LEU9P
@> ASP92P  <--->  hb:ARG18P  sb:ARG18P  hb:ASN95P  hb:LEU96P
@> ASP98P  <--->  hb:ARG101P  sb:ARG101P  hb:LYS102P  hb:LYS102P  sb:LYS102P  hb:SER94P
@> LYS102P  <--->  rb:ARG101P  hb:GLN105P  hp:ILE77P  hb:ASP98P  hb:ASP98P  sb:ASP98P
@> LYS112P  <--->  hb:ILE88P  sb:GLU114P  pc:HIS157P  hb:ASP86P  hb:HIS157P
@> GLU114P  <--->  hb:CYS90P  hb:ILE88P  sb:LYS112P  sb:HIS157P
@> TYR119P  <--->  hb:HIS157P  hp:LEU89P  hb:HIS157P  ps:HIS157P
@> ASP120P  <--->  hb:LYS123P  hb:GLN124P  sb:ARG147P  hb:GLY117P
@> ILE127P  <--->  hb:ARG18P  hp:MET91P  hp:LEU116P  hp:VAL141P  hb:MET91P
@> TYR131P  <--->  hb:ARG58P  hb:ARG58P  ps:TYR132P  hp:ILE16P
@> PHE138P  <--->  hp:ARG58P  hb:TYR142P  hp:ILE21P  hb:ASN134P
@> GLU139P  <--->  hb:ARG65P  hb:HIS66P  sb:HIS66P  hb:GLN143P  hb:GLN143P  sb:ARG65P  hb:ASP135P
@> VAL141P  <--->  hp:ARG18P  hb:CYS145P  hp:ILE127P  hb:ASP137P
@> TYR142P  <--->  hp:VAL25P  hb:VAL146P  ps:HIS66P  hb:PHE138P  hp:VAL146P
@> ARG147P  <--->  hb:ALA151P  sb:ASP120P  hb:GLN124P  hb:GLN124P  hb:GLN143P
@> HIS157P  <--->  hb:LYS112P  sb:GLU114P  hb:TYR119P  ps:TYR119P  pc:LYS112P  hb:TYR119P
@> ARG101P  <--->  hb:ARG97P  hb:ASP98P  sb:ASP98P  rb:LYS102P
@>
Legend: hb-hydrogen bond, sb-salt bridge, rb-repulsive ionic bond, ps-Pi stacking interaction,
pc-Cation-Pi interaction, hp-hydrophobic interaction, dibs-disulfide bonds
```

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

In [20]: showProteinInteractions_VMD(atoms, interactions.getSaltBridges(),
   ....:                                    color='yellow',filename='SBs.tcl')
   ....:

In [21]: showProteinInteractions_VMD(atoms, interactions.getRepulsiveIonicBonding(),
   ....:                                    color='red',filename='RIB.tcl')
   ....:

In [22]: showProteinInteractions_VMD(atoms, interactions.getPiStacking(),
   ....:                                    color='green',filename='PiStacking.tcl')
   ....:

In [23]: showProteinInteractions_VMD(atoms, interactions.getPiCation(),
   ....:                                    color='orange',filename='PiCation.tcl')
   ....:

In [24]: showProteinInteractions_VMD(atoms, interactions.getHydrophobic(),
   ....:                                    color='silver',filename='HPh.tcl')
   ....:

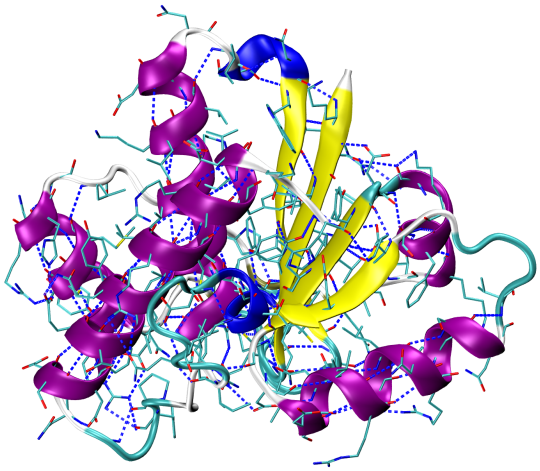
In [25]: showProteinInteractions_VMD(atoms, interactions.getDisulfideBonds(),
   ....:                                    color='black',filename='DiBs.tcl')
   ....:
```

```
@> 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:

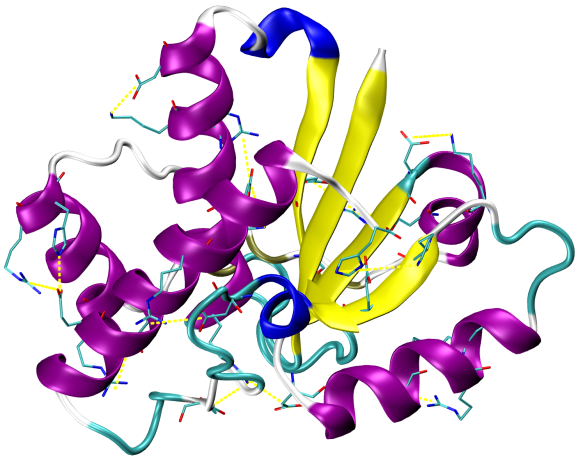
```
play HBs.tcl
```

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.



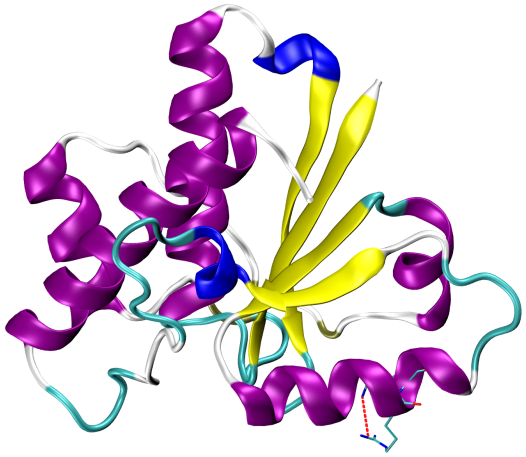
Salt bridges in yellow (**VMD_** *TK Console*):

```
play SBs.tcl
```



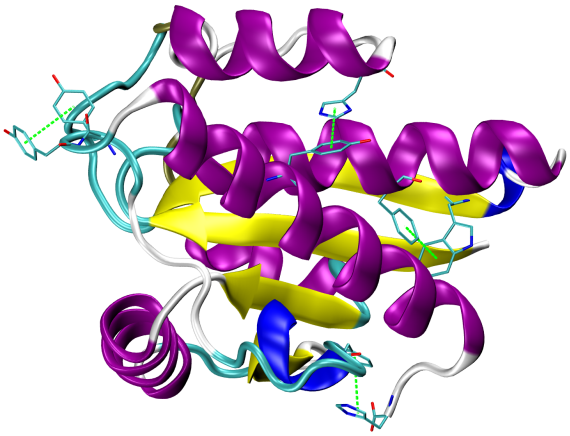
Repulsive ionic bonding in red (**VMD_** *TK Console*):

```
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*):

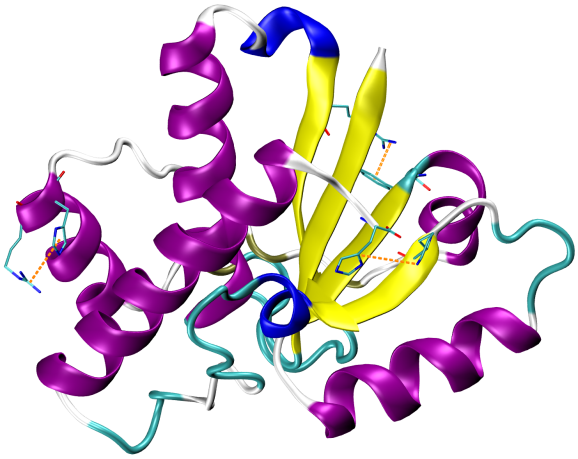
```
play HPh.tcl
```

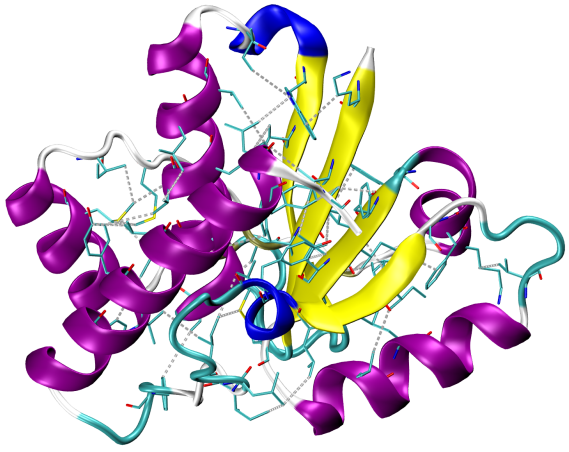
2.4 Additional selections

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 [26]: 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 [27]: interactions.getRepulsiveIonicBonding(selection='resid 102')
```

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

```
In [28]: 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 [29]: allRes_20to50 = interactions.getInteractions(selection='resid 20 to 50')

In [30]: 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 [31]: 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 [32]: 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 [33]: interactions.getPiCation(selection='resid 85')
```

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

```
In [34]: 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 [35]: newHydrogenBonds2 = calcHydrogenBonds(atoms, distA=2.8,
   ....:                                angle=30, cutoff_dist=15)
   ....:

In [36]: 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 [37]: 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 [38]: sb2 = calcSaltBridges(atoms, distA=6)

In [39]: interactions.setNewSaltBridges(sb2)

In [40]: rib2 = calcRepulsiveIonicBonding(atoms, distA=9)

In [41]: interactions.setNewRepulsiveIonicBonding(rib2)

In [42]: picat2 = calcPiCation(atoms, distA=7)

In [43]: 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 [44]: matrix = interactions.buildInteractionMatrix()
```

```
@> Calculating interactions
```

The results can be displayed in the following way:

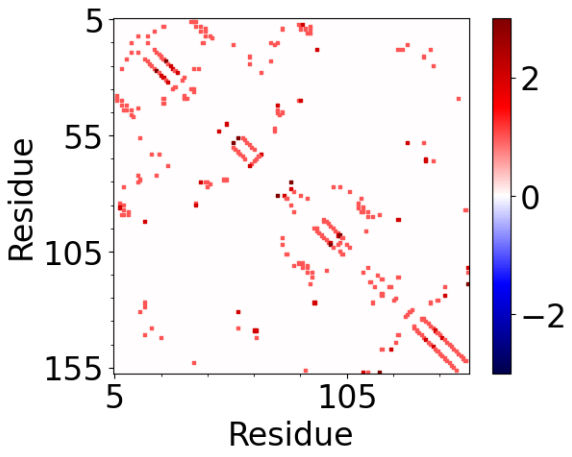
```
In [45]: import matplotlib.pylab as plt

In [46]: showAtomicMatrix(matrix, atoms=atoms.ca, cmap='seismic', markersize=5)

In [47]: plt.xlabel('Residue')
```

```
In [48]: plt.ylabel('Residue')

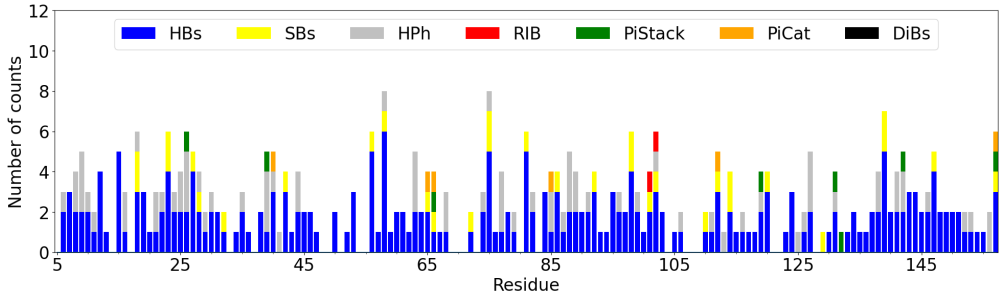
In [49]: plt.clim([-3,3])
```



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

```
In [50]: interactions.showCumulativeInteractionTypes()
```

```
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
```



2.7 Energy of interactions

Additionally, we can also obtain energy of the pairs of identified interactions with several functions. One of them is `showPairEnergy()` method that will check the energy of interactions for pairs of residues and add it to the interactions list. Energies will be added at the last position for each pair.

```
In [51]: showPairEnergy(interactions.getHydrogenBonds())
```

```
[['ARG101', 'NH1_1516', 'P', 'ASP98', 'OD1_1463', 'P', 1.998, 33.1238, -3.92],
['HIS72', 'NE2_1042', 'P', 'ASN15', 'OD1_165', 'P', 2.5997, 34.752, -3.05],
['GLN143', 'NE2_2192', 'P', 'GLU139', 'OE2_2126', 'P', 2.7287, 9.1823, -3.45],
```

```
['HIS66', 'NE2_957', 'P', 'GLU139', 'OE1_2125', 'P', 2.7314, 6.3592, -3.15],
['ARG40', 'N_561', 'P', 'LYS6', 'O_37', 'P', 2.7479, 17.1499, -2.11],
['ARG58', 'N_813', 'P', 'ASP56', 'OD1_788', 'P', 2.7499, 29.9737, -3.92],
['ALA45', 'N_634', 'P', 'ARG75', 'O_1097', 'P', 2.7609, 35.0983, -3.26],
['ASN53', 'ND2_747', 'P', 'GLU50', 'OE1_708', 'P', 2.7702, 18.2336, -2.43],
['ALA74', 'N_1064', 'P', 'ASN53', 'O_751', 'P', 2.7782, 21.3375, -2.06],
['ASP56', 'N_780', 'P', 'ILE16', 'O_189', 'P', 2.7793, 27.0481, -3.46],
['LYS110', 'NZ_1667', 'P', 'THR84', 'O_1240', 'P', 2.7977, 38.2213, -1.64],
['LEU116', 'N_1758', 'P', 'CYS90', 'O_1342', 'P', 2.8072, 15.0239, -6.13],
['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 2.8075, 29.107, -4.12],
['ASN134', 'N_2045', 'P', 'ASP137', 'OD2_2091', 'P', 2.8132, 22.562, -2.5],
['PHE152', 'N_2321', 'P', 'CYS148', 'O_2275', 'P', 2.8141, 8.2562, -4.81],
['ASN95', 'N_1398', 'P', 'ASP92', 'OD1_1368', 'P', 2.8148, 12.5701, -2.5],
['LYS6', 'N_16', 'P', 'ASN38', 'O_536', 'P', 2.8178, 25.0305, -1.63],
['ILE77', 'N_1115', 'P', 'ALA45', 'O_643', 'P', 2.8179, 12.1855, -4.45],
['ARG58', 'NH2_832', 'P', 'ASP56', 'OD2_789', 'P', 2.8204, 27.6617, -3.92],
['LEU99', 'N_1467', 'P', 'ASN95', 'O_1411', 'P', 2.8205, 15.4867, -3.94],
['CYS149', 'N_2276', 'P', 'CYS145', 'O_2224', 'P', 2.8247, 9.5914, -7.23],
['GLY52', 'N_731', 'P', 'ALA74', 'O_1073', 'P', 2.832, 6.6442, -2.24],
['ASP32', 'N_435', 'P', 'LYS28', 'O_385', 'P', 2.8357, 8.8318, -2.47],
['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.8429, 17.7147, -2.88],
..
..
```

Another function is `Interactions.buildInteractionMatrixEnergy()` which provides matrix with energies of interactions for each pair.

```
In [52]: matrix_en = interactions.buildInteractionMatrixEnergy()
```

```
@> Calculating interaction matrix
```

The results can be displayed in the following way:

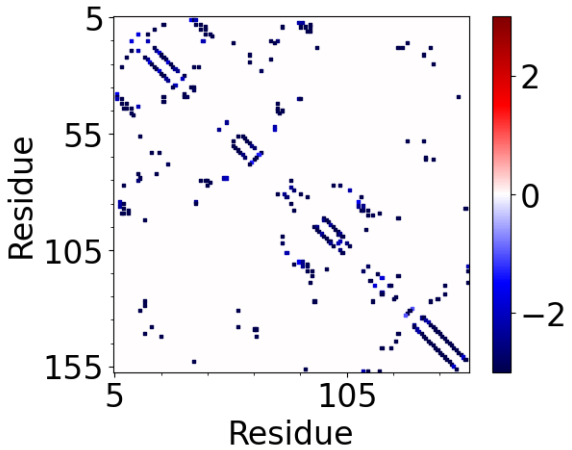
```
In [53]: import matplotlib.pylab as plt

In [54]: showAtomicMatrix(matrix_en, atoms=atoms.ca, cmap='seismic', markersize=5)

In [55]: plt.xlabel('Residue')

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

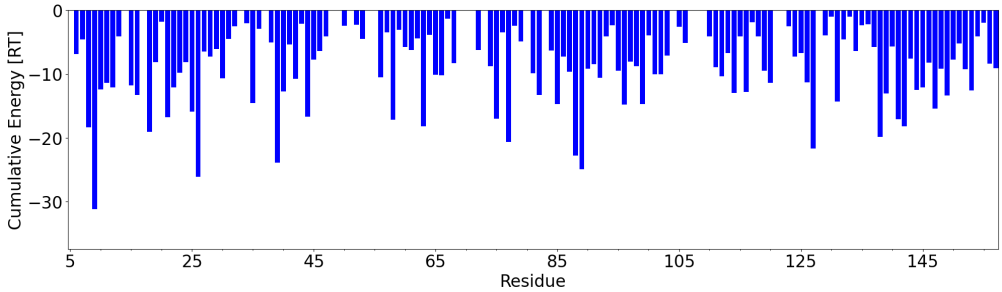
In [57]: plt.clim([-3,3])
```



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

```
In [58]: interactions.showCumulativeInteractionTypes(energy=True)
```

```
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
```



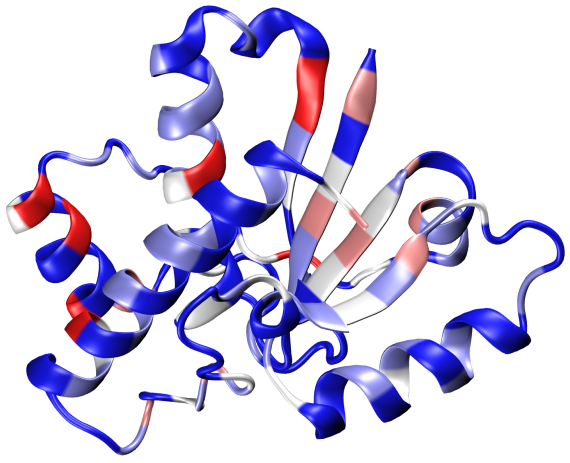
2.8 Visualize number of interactions onto 3D structure

The number of the interaction or total energy 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 [59]: 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*.



To save energy of interaction instead of number of interactions we can use the following command:

```
In [60]: interactions.saveInteractionsPDB(filename='5kqm_meanMatrix_en.pdb', energy=True)
```

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

2.9 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 [61]: matrix = interactions.buildInteractionMatrix(RIB=0, HBs=0, HPh=0, DiBs=0)
```

```
@> Calculating interaction matrix
```

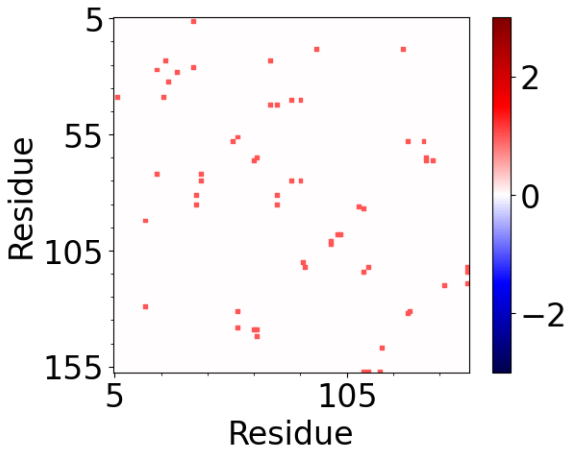
The results can be displayed in a similar way:

```
In [62]: showAtomicMatrix(matrix, atoms=atoms.ca, cmap='seismic', markersize=8)

In [63]: plt.xlabel('Residue')

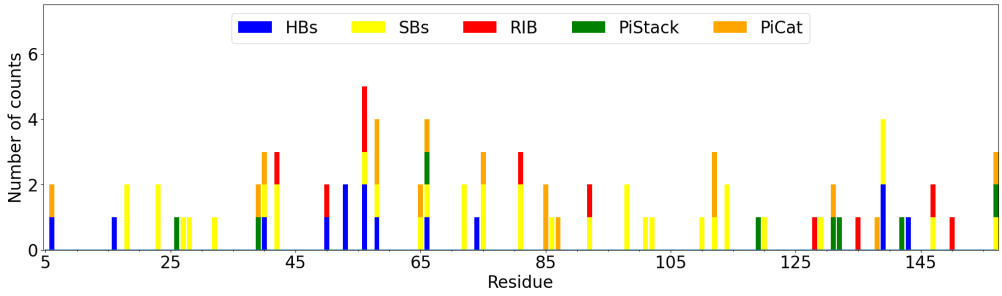
In [64]: plt.ylabel('Residue')

In [65]: plt.clim([-3,3])
```




```
In [66]: interactions.showCumulativeInteractionTypes(HPh=0, DiBs=0)
```

```
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
```


HBs
SBs
RIB
PiStack
PiCat
Number of counts
0
2
4
6
5
25
45
65
85
105
125
145
Residue

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)
```

```
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 5kqm downloaded (5kqm.pdb)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
```

[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.
```

4.2 Perform InSty calculations and extract chain-chain interactions

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

4.3 Compute Interactions

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
```

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

@>	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
@>	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

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@>     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
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@>     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
@>     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
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@>     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
@>     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_6960
```

```
@>     HIS227       A        1719_1720_1721_1722_1723  <--->     HIS231       A        1754_1755_1756
@>     PHE640       A   4970_4971_4972_4973_4974_4975  <--->     PHE487       A   3788_3789_3790_3791
@>     HIS411       B        8382_8383_8384_8385_8386  <--->     TYR176       B   6507_6508_6509_6510
@>     TRP566       B   9609_9611_9612_9613_9614_9615  <--->     PHE229       B   6938_6939_6940_6941
@>     PHE640       B10174_10175_10176_10177_10178_10179  <--->     PHE487       B   8992_8993_8994_8
@>     HIS373       B        8063_8064_8065_8066_8067  <--->     HIS378       B        8105_8106_8107
@>     PHE229       A   1734_1735_1736_1737_1738_1739  <--->     TRP566       A   4405_4407_4408_4409
@>     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.
```

4.4 Select interactions between chains

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')
```

```
[]
```

4.5 Set only interactions between chains

With the above functions, we can display particular types of interactions between selected chains. To set this selection and ignore all intramolecular interactions, we can use `replace` option.

```
In [12]: chain_interactions = interactions.getInteractions(selection='chain A', selection2='chain B',
   ....:                                                   replace=True)
   ....:
```

```
@> New interactions are set
```

```
In [13]: chain_interactions
```

```
[[['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]],
 [['ARG215', 'NH1_1619_1620', 'A', 'GLU168', 'OE1_6442_6443', 'B', 2.6066],
  ['ARG208', 'NH1_1560_1561', 'A', 'GLU111', 'OE1_5976_5977', 'B', 4.3468]],
 [],
 [],
 [],
 [['ILE197', 'CD1_1467', 'A', 'PHE184', 'CD2_6569', 'B', 3.2502, 29.5284],
  ['LEU419', 'CD1_8449', 'B', 'LYS196', 'CD_1457', 'A', 3.4645, 34.5683],
  ['ILE197', 'CD1_6671', 'B', 'ALA182', 'CB_1349', 'A', 3.7348, 34.1782],
  ['LEU186', 'CD1_1387', 'A', 'ALA193', 'CB_6637', 'B', 4.2965, 20.2503]],
 []]
```

Now, when new interactions are set, we can use the functions that we introduced before:

Interaction matrix:

```
In [14]: matrix = interactions.buildInteractionMatrix()
```

```
@> Calculating interaction matrix
```

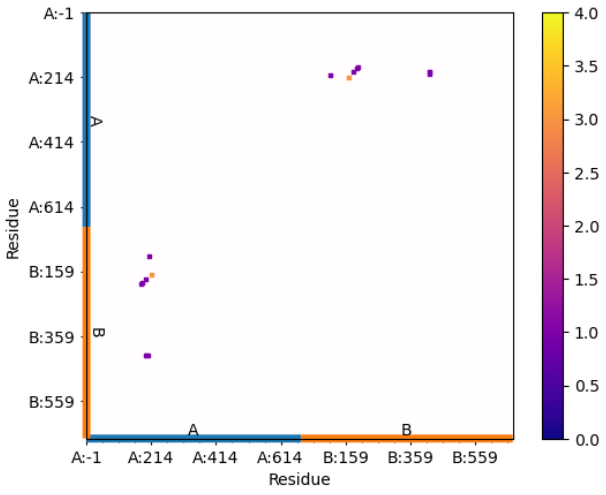
```
In [15]: import matplotlib.pylab as plt

In [16]: showAtomicMatrix(matrix, atoms=atoms.ca, cmap='plasma', markersize=5)

In [17]: plt.xlabel('Residue')

In [18]: plt.ylabel('Residue')

In [19]: plt.clim([0,np.max(matrix)+1])
```



Interaction matrix displayed with energies:

```
In [20]: matrix_en = interactions.buildInteractionMatrixEnergy()
```

```
@> Calculating interaction energies matrix with type IB_solv
```

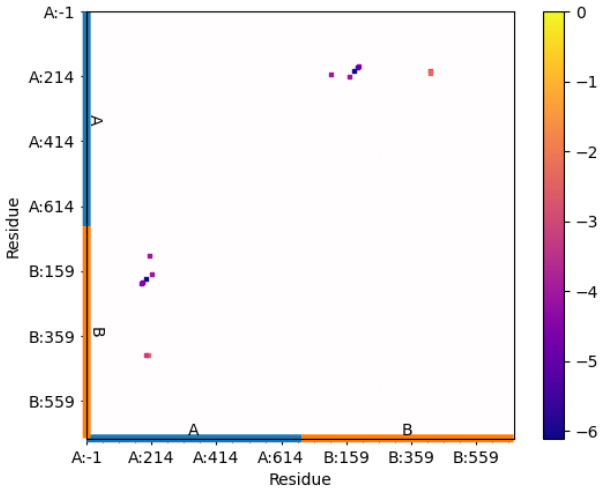
```
In [21]: import matplotlib.pylab as plt

In [22]: showAtomicMatrix(matrix_en, atoms=atoms.ca, cmap='plasma',
   ....:                  markersize=5)
   ....:

In [23]: plt.xlabel('Residue')

In [24]: plt.ylabel('Residue')

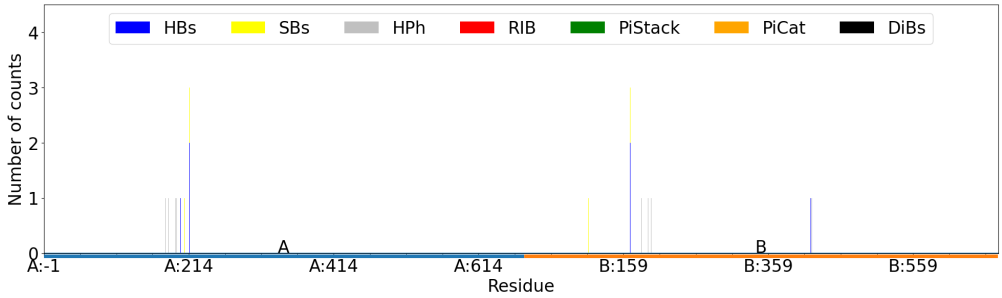
In [25]: plt.clim([np.min(matrix_en),0])
```



A bar plot with information about interaction types per residue between the two chains:

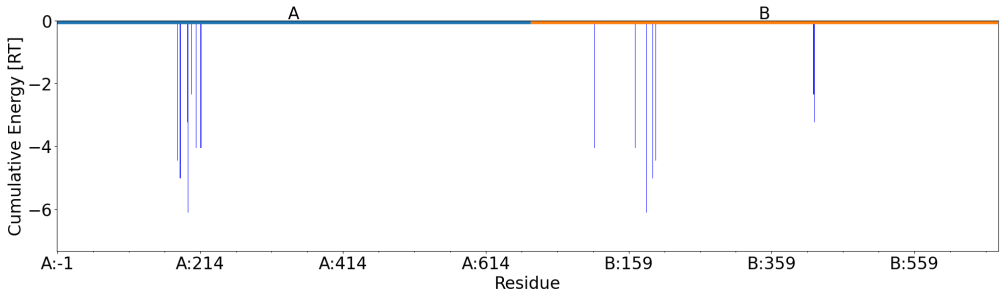
```
In [26]: interactions.showCumulativeInteractionTypes()
```

```
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
```



A bar plot with information about interaction types per residue between the two chains displayed by energies instead of the interactions number:

```
In [27]: interactions.showCumulativeInteractionTypes(energy=True)
```



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 [28]: interactions.saveInteractionsPDB(filename='7laf_meanMatrix_chAB_both.pdb')
```

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

Also, with enegies instead of the number of interactions:

```
In [29]: interactions.saveInteractionsPDB(filename='7laf_meanMatrix_chAB_both_en.pdb', energy=True)
```

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

We can also save all the interactions into the TCL scripts to visualize them in VMD_.

```
In [30]: showProteinInteractions_VMD(atoms, interactions.getHydrogenBonds(),
   ....:                                color='blue', filename='7laf_HBs_chAB.tcl')
   ....:

In [31]: showProteinInteractions_VMD(atoms, interactions.getSaltBridges(),
   ....:                                color='yellow',filename='7laf_SBs_chAB.tcl')
   ....:

In [32]: showProteinInteractions_VMD(atoms, interactions.getRepulsiveIonicBonding(),
   ....:                                color='red',filename='7laf_RIB_chAB.tcl')
   ....:

In [33]: showProteinInteractions_VMD(atoms, interactions.getPiStacking(),
   ....:                                color='green',filename='7laf_PiStacking_chAB.tcl')
   ....:

In [34]: showProteinInteractions_VMD(atoms, interactions.getPiCation(),
   ....:                                color='orange',filename='7laf_PiCation_chAB.tcl')
   ....:

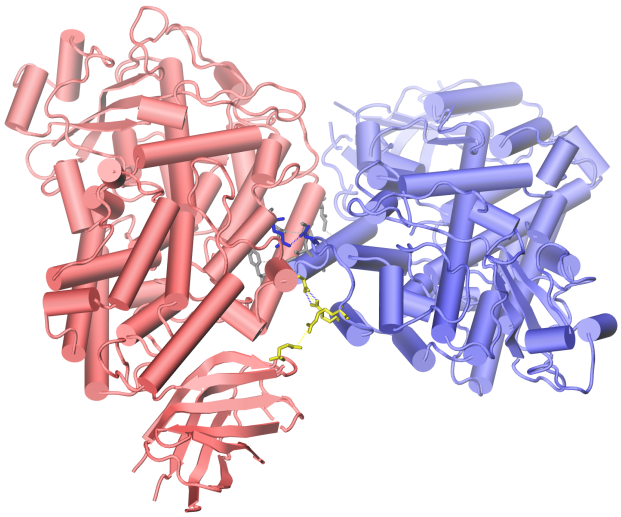
In [35]: showProteinInteractions_VMD(atoms, interactions.getHydrophobic(),
   ....:                                color='silver',filename='7laf_HPh_chAB.tcl')
   ....:

In [36]: showProteinInteractions_VMD(atoms, interactions.getDisulfideBonds(),
   ....:                                color='black',filename='7laf_DiBs_chAB.tcl')
   ....:
```

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

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

After uploading `TCL` scripts to VMD, as it was explained before, we can obtain such a view:



Except for visualization, we can also get access to the most frequent interactors, i.e., residues that can form the biggest number of possible interactions.

```
In [37]: interactions.getFrequentInteractors()
```

```
@> GLU168B  <--->  hb:ARG215A  hb:ARG215A  sb:ARG215A
@> ARG215A  <--->  hb:GLU168B  hb:GLU168B  sb:GLU168B
@>
Legend: hb-hydrogen bond, sb-salt bridge, rb-repulsive ionic bond, ps-Pi stacking interaction,
pc-Cation-Pi interaction, hp-hydrophobic interaction, dibs-disulfide bonds
```

To have access to interactors that are having smaller number of interactions, we can modify `contacts_min` parameter.

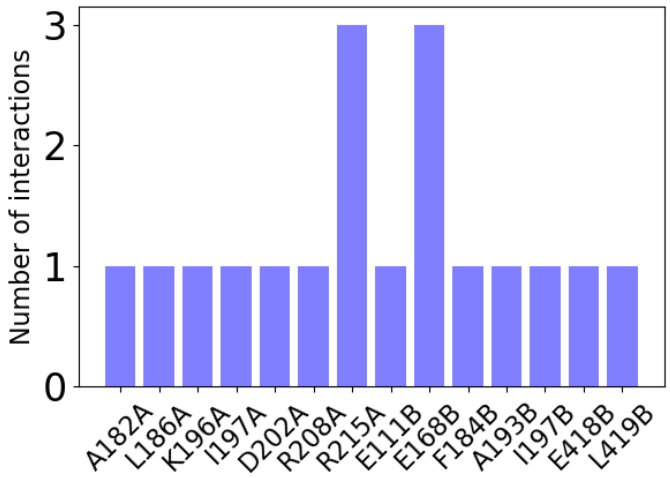
```
In [38]: interactions.getFrequentInteractors(contacts_min=1)
```

```
@> ALA182A  <--->  hp:ILE197B
@> LYS196A  <--->  hp:LEU419B
@> GLU111B  <--->  sb:ARG208A
@> GLU168B  <--->  hb:ARG215A  hb:ARG215A  sb:ARG215A
@> PHE184B  <--->  hp:ILE197A
@> ALA193B  <--->  hp:LEU186A
@> GLU418B  <--->  hb:ASP202A
@> ILE197B  <--->  hp:ALA182A
@> LEU419B  <--->  hp:LYS196A
@> ARG208A  <--->  sb:GLU111B
@> ARG215A  <--->  hb:GLU168B  hb:GLU168B  sb:GLU168B
@> ILE197A  <--->  hp:PHE184B
```

```
@> LEU186A  <--->  hp:ALA193B
@> ASP202A  <--->  hb:GLU418B
@>
Legend: hb-hydrogen bond, sb-salt bridge, rb-repulsive ionic bond, ps-Pi stacking interaction,
pc-Cation-Pi interaction, hp-hydrophobic interaction, dibs-disulfide bonds
```

We can also diplay them as a bar plot:

```
In [39]: interactions.showFrequentInteractors(cutoff = 1)
```



To have access to information about the type of possible interactions and residue partner, we can use the `getInteractors()` function and define residue by its three letter code and chain ID.

```
In [40]: interactions.getInteractors('ARG215A')
```

```
@> hb:ARG215A-GLU168B
@> hb:ARG215A-GLU168B
@> sb:ARG215A-GLU168B
```

CHAPTER

FIVE

EXTRACT CHAIN-CHAIN INTERACTIONS IN ENSEMBLE OR TRAJECTORY ANALYSIS

To extract the intermolecular interactions between two chains in a trajectory or PDB ensemble, we should follow the corresponding tutorial and include selections (`selection` and `selection2`) and the `replace` parameter set to `True` as follows:

```
In [41]: interactionsTrajectory.getInteractions(selection='chain A', selection2='chain B', replace=Tr
```

Once we use `replace = True`, the selection will be replaced by chain-chain interactions or any other interaction selected by selecting option. Be aware that once `replace` is used, you can not return back to all interactions.

CHAPTER

SIX

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.

6.1 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.
```

6.2 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.
..
..
```

6.3 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_1
@> 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_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: 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_8
@> 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.
```

6.4 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, `calcProteinInteractionsEnsemblePDB.pkl` can be reloaded and used with all available functions and methods.

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

In [13]: interactionsTrajectoryNMR.calcProteinInteractionsTrajectory(atoms,
   ....: filename='calcProteinInteractionsEnsemblePDB.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
```

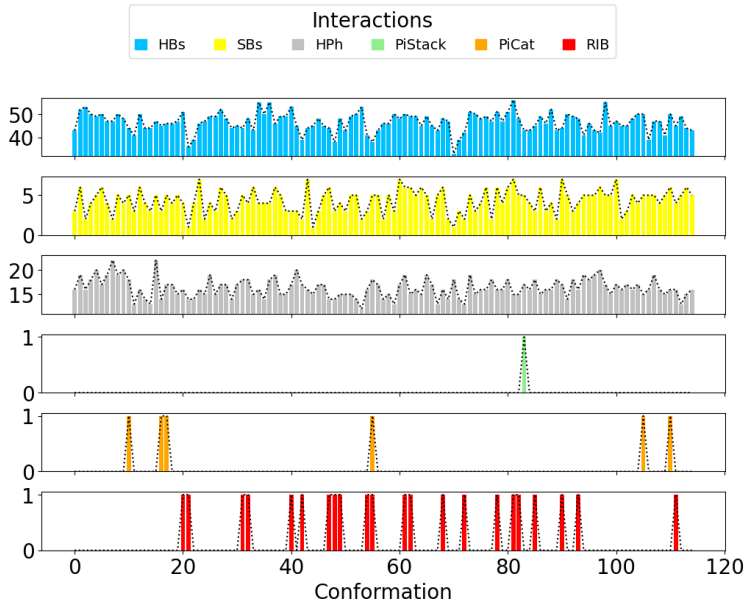
```
@>      VAL26    A         N_400  <--->      THR22    A         O_341     3.4    23.5
@>      GLN41    A         N_638  <--->      PRO38    A         O_598     3.4    34.4
@>      ILE23    A         N_352  <--->      ARG54    A         O_849     3.5    23.1
@>      ASN60    A         N_947  <--->      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
@>   Energy [RT]: -2.83
@> Statistics for GLY10A-THR7A:
@>   Average [Ang.]: 3.037245
@>   Standard deviation [Ang.]: 0.1988
```

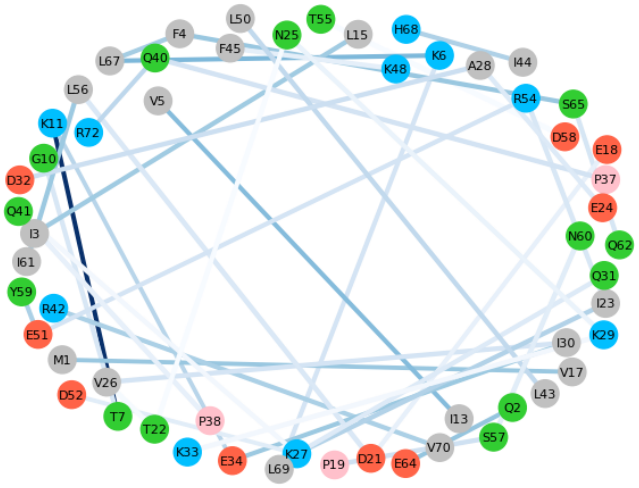
```
@>   Weight: 0.669565
@>   Energy [RT]: -1.81
@> Statistics for ARG72A-GLN40A:
@>   Average [Ang.]: 2.874946
@>   Standard deviation [Ang.]: 0.18885
@>   Weight: 0.782609
@>   Energy [RT]: -4.13
@> Statistics for LYS6A-LEU67A:
@>   Average [Ang.]: 2.920333
@>   Standard deviation [Ang.]: 0.157525
@>   Weight: 0.947826
@>   Energy [RT]: -3.24
@> Statistics for GLU34A-ILE30A:
@>   Average [Ang.]: 2.896524
@>   Standard deviation [Ang.]: 0.171493
@>   Weight: 0.878261
@>   Energy [RT]: -3.99
@> Statistics for THR55A-ASP58A:
@>   Average [Ang.]: 2.777835
@>   Standard deviation [Ang.]: 0.158068
@>   Weight: 1.504348
@>   Energy [RT]: -2.41
@> Statistics for ILE44A-HIS68A:
@>   Average [Ang.]: 2.941125
@>   Standard deviation [Ang.]: 0.177848
@>   Weight: 0.834783
@>   Energy [RT]: -4.55
@> Statistics for LYS29A-ASN25A:
@>   Average [Ang.]: 3.050209
@>   Standard deviation [Ang.]: 0.211243
@>   Weight: 0.582609
@>   Energy [RT]: -1.63
@> Statistics for HIS68A-ILE44A:
@>   Average [Ang.]: 2.951679
@>   Standard deviation [Ang.]: 0.195428
@>   Weight: 0.826087
@>   Energy [RT]: -4.55
@> Statistics for GLU51A-TYR59A:
@>   Average [Ang.]: 2.967038
@>   Standard deviation [Ang.]: 0.18416
@>   Weight: 0.834783
@>   Energy [RT]: -3.62
@> Statistics for GLU64A-GLN2A:
@>   Average [Ang.]: 2.860456
@>   Standard deviation [Ang.]: 0.142289
@>   Weight: 0.895652
@>   Energy [RT]: -3.45
@> Statistics for LEU50A-LEU43A:
@>   Average [Ang.]: 3.028411
@>   Standard deviation [Ang.]: 0.19173
@>   Weight: 0.773913
@>   Energy [RT]: -7.16
@> Statistics for ILE13A-VAL5A:
@>   Average [Ang.]: 2.900624
@>   Standard deviation [Ang.]: 0.149592
@>   Weight: 0.930435
@>   Energy [RT]: -5.31
@> Statistics for SER65A-GLN62A:
```

```
@>   Average [Ang.]: 2.989405
@>   Standard deviation [Ang.]: 0.276179
@>   Weight: 0.678261
@>   Energy [RT]: -3.06
@> Statistics for VAL17A-MET1A:
@>   Average [Ang.]: 2.917662
@>   Standard deviation [Ang.]: 0.146237
@>   Weight: 0.93913
@>   Energy [RT]: -5.16
@> Statistics for ASN60A-SER57A:
@>   Average [Ang.]: 3.176033
@>   Standard deviation [Ang.]: 0.176174
@>   Weight: 0.626087
@>   Energy [RT]: -2.13
..
..
```

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.

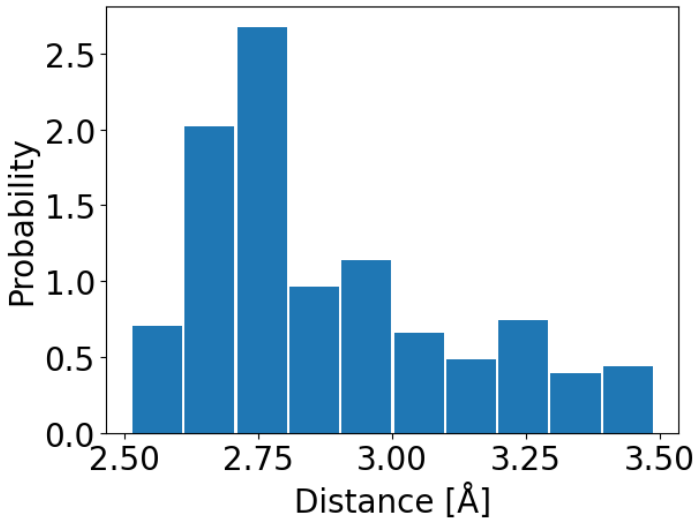
```
In [16]: showInteractionsGraph(statistics, code='1-letter', cutoff=0.5,
   ....:                                                font_size=8, seed=42)
   ....:
```



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
```

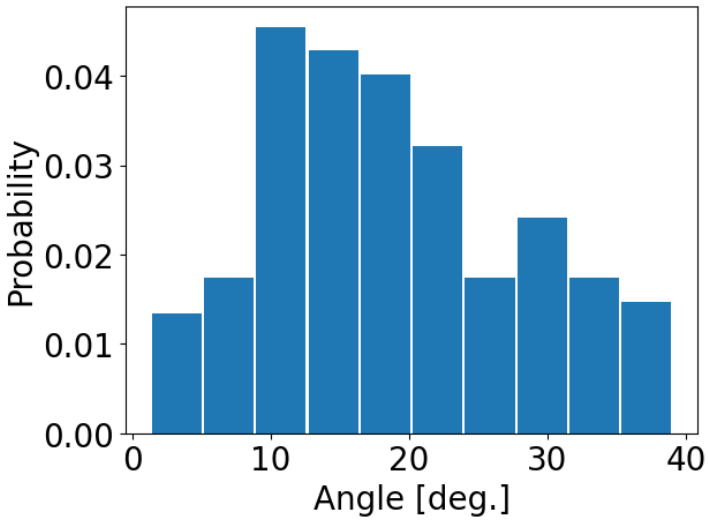
We will obtain a histogram with distances for *LYS11* residue and information about other contact residues for this particular residue.

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')
```

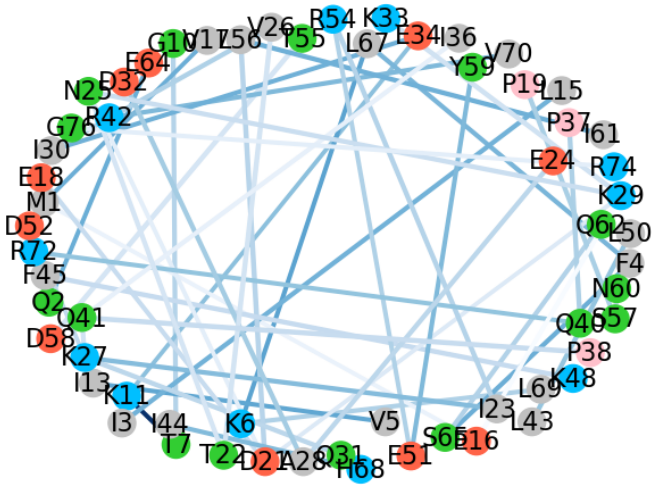


```
@> Additional contacts for LYS11:
@> GLY76
@> GLU34
@> LEU73
```

6.5 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')

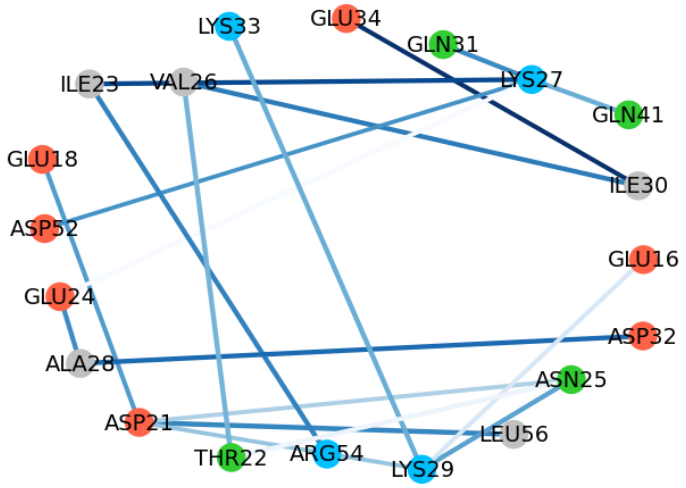
In [23]: statistics2 = calcStatisticsInteractions(hbs_20to30)

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.
```

6.6 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],
   ..
   ..
```

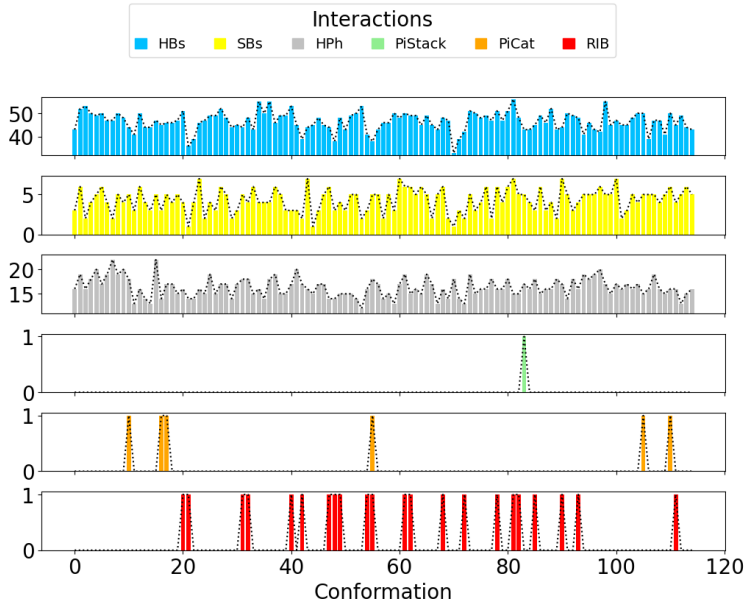
After parsing the file we will have access to the same functions as before:

```
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()
```



6.7 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

SEVEN

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).

7.1 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.
..
..
```

7.2 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
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@>      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
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@>      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
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@>      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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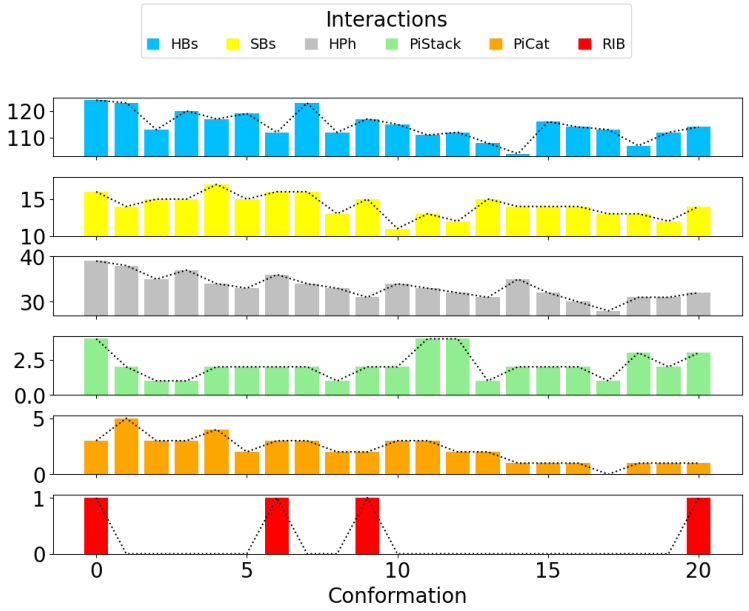
Moreover, we can display the evolution of each interaction type during the simulation. There are the following types of plots: hydrogen bonds (*blue*), salt bridges (*yellow*), hydrophobic interactions (*silver*), Pi-stacking (*green*), Pi-cation (*orange*), repulsive ionic bonding (*red*), disulfide 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],
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In [19]: interactionsTrajectory.getSaltBridges()
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[[['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],
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  ['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],
  ..
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```

```
In [20]: interactionsTrajectory.getHydrophobic()
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[[['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],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD2_1464', 'P', 2.8351, 14.4292],
  ['ARG101', 'NE_1513', 'P', 'ASP98', 'OD1_1463', 'P', 2.8423, 25.7739],
  ['ARG101', 'NH2_1519', 'P', 'ASP98', 'OD1_1463', 'P', 2.8761, 36.221],
  ['ASN100', 'N_1486', 'P', 'LEU96', 'O_1430', 'P', 2.9016, 29.2602],
  ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 2.9501, 21.9519],
  ['LYS102', 'N_1524', 'P', 'ASP98', 'O_1466', 'P', 2.9534, 4.572],
  ['VAL106', 'N_1588', 'P', 'LYS102', 'O_1545', 'P', 2.9715, 13.2817],
  ['ASN104', 'N_1557', 'P', 'ASN100', 'O_1499', 'P', 3.0385, 28.4861],
  ['GLN105', 'N_1571', 'P', 'ARG101', 'O_1523', 'P', 3.0741, 22.6725],
  ['ARG101', 'N_1500', 'P', 'ARG97', 'O_1454', 'P', 3.0961, 21.9463]],
 [['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD2_1464', 'P', 2.6673, 5.897],
  ['ARG101', 'NE_1513', 'P', 'ASP98', 'OD2_1464', 'P', 2.8621, 21.3715],
  ['ARG101', 'NH2_1519', 'P', 'ASP98', 'OD2_1464', 'P', 2.9062, 37.2809],
  ['SER103', 'OG_1553', 'P', 'LEU99', 'O_1485', 'P', 2.9467, 14.2625],
  ['LYS102', 'N_1524', 'P', 'ASP98', 'O_1466', 'P', 3.0105, 15.1965],
  ['ASN100', 'N_1486', 'P', 'LEU96', 'O_1430', 'P', 3.1835, 33.0481],
  ['GLN105', 'N_1571', 'P', 'ARG101', 'O_1523', 'P', 3.2504, 29.8412],
  ['VAL106', 'N_1588', 'P', 'LYS102', 'O_1545', 'P', 3.4557, 26.8981]],
 [['ARG101', 'NE_1513', 'P', 'ASP98', 'OD1_1463', 'P', 2.6955, 15.9473],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463', 'P', 2.7336, 13.04],
  ['SER103', 'OG_1553', 'P', 'LEU99', 'O_1485', 'P', 2.7844, 21.0059],
  ['ASN100', 'N_1486', 'P', 'LEU96', 'O_1430', 'P', 2.7921, 34.0413],
  ['ASN104', 'N_1557', 'P', 'ASN100', 'O_1499', 'P', 2.8616, 30.9582],
  ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 2.9622, 35.633],
  ['LYS102', 'N_1524', 'P', 'ASP98', 'O_1466', 'P', 2.9862, 9.5713],
  ['ARG101', 'NH2_1519', 'P', 'ASP98', 'OD2_1464', 'P', 2.992, 28.725],
  ['ARG101', 'NH2_1519', 'P', 'ASP98', 'OD1_1463', 'P', 3.0439, 38.4803],
  ['ARG101', 'N_1500', 'P', 'ARG97', 'O_1454', 'P', 3.2289, 6.3339],
  ['GLN105', 'N_1571', 'P', 'ARG101', 'O_1523', 'P', 3.3376, 16.6525],
  ['VAL106', 'N_1588', 'P', 'LYS102', 'O_1545', 'P', 3.3409, 32.703]],
 [['SER103', 'OG_1553', 'P', 'LEU99', 'O_1485', 'P', 2.6495, 18.2239],
  ['ARG101', 'NE_1513', 'P', 'ASP98', 'OD1_1463', 'P', 2.675, 14.3671],
  ['ASN100', 'N_1486', 'P', 'LEU96', 'O_1430', 'P', 2.6999, 16.6616],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463', 'P', 2.7186, 10.5368],
  ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 2.8422, 23.6928],
  ['ASN104', 'N_1557', 'P', 'ASN100', 'O_1499', 'P', 2.8537, 21.8508],
  ['LYS102', 'N_1524', 'P', 'ASP98', 'O_1466', 'P', 2.8826, 12.651],
  ['ARG101', 'N_1500', 'P', 'ARG97', 'O_1454', 'P', 2.9711, 26.7601],
  ['GLN105', 'N_1571', 'P', 'ARG101', 'O_1523', 'P', 3.1186, 14.3141],
  ['VAL106', 'N_1588', 'P', 'LYS102', 'O_1545', 'P', 3.2655, 29.3262]],
 [['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD2_1464', 'P', 2.6587, 11.1386],
  ['ARG101', 'NH2_1519', 'P', 'ASP98', 'OD2_1464', 'P', 2.7047, 15.6631],
  ['ASN100', 'N_1486', 'P', 'LEU96', 'O_1430', 'P', 2.791, 11.1184],
  ['GLN105', 'N_1571', 'P', 'ARG101', 'O_1523', 'P', 2.801, 22.9498],
  ['ARG101', 'NE_1513', 'P', 'ASP98', 'OD2_1464', 'P', 2.9519, 31.5282],
```

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  ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 3.0148, 11.0913],
  ['ARG101', 'N_1500', 'P', 'ARG97', 'O_1454', 'P', 3.3007, 38.2386],
  ['LYS102', 'N_1524', 'P', 'ASP98', 'O_1466', 'P', 3.3317, 21.1],
  ['VAL106', 'N_1588', 'P', 'LYS102', 'O_1545', 'P', 3.4041, 33.0264]],
 [['ARG101', 'NH2_1519', 'P', 'ASP98', 'OD2_1464', 'P', 2.5558, 15.1737],
  ['ARG101', 'NE_1513', 'P', 'ASP98', 'OD2_1464', 'P', 2.7324, 21.7444],
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  ['ARG101', 'N_1500', 'P', 'ARG97', 'O_1454', 'P', 3.271, 31.13],
  ['CYS109', 'SG_1647', 'P', 'SER103', 'OG_1553', 'P', 3.3052, 14.7978]],
 [['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD2_1464', 'P', 2.671, 37.3323],
  ['ARG101', 'NH2_1519', 'P', 'ASP98', 'OD2_1464', 'P', 2.739, 34.0943],
  ['ARG101', 'NE_1513', 'P', 'ASP98', 'OD2_1464', 'P', 2.7588, 35.9299],
  ['ASN100', 'N_1486', 'P', 'LEU96', 'O_1430', 'P', 2.8159, 18.3284],
  ['ASN100', 'ND2_1495', 'P', 'LEU96', 'O_1430', 'P', 2.8621, 29.9939],
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  ['ARG101', 'NH2_1519', 'P', 'ASP98', 'OD1_1463', 'P', 2.8136, 16.1535],
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[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 2.9739],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.3131]],
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 [['LYS79', 'CG_1155', 'P', 'VAL106', 'CG1_1594', 'P', 3.7466, 15.362],
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 [['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]],
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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],
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  ['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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  ['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]],
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  ['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]],
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  ['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],
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  ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.089, 17.9789]],
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  ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.0718, 34.4381],
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 [['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],
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  ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.2056, 13.0868]],
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  ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.8455, 10.8341],
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  ['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]],
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  ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 3.0654, 16.9354],
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  ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.833, 1.7101],
  ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.9604, 20.771],
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  ['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]]]
```

7.3 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
```

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@>      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]],
   ..
   ..
```

7.4 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
@>   Energy [RT]: -4.51
@> Statistics for HIS66P-ARG65P:
@>   Average [Ang.]: 4.717772006988525
@>   Standard deviation [Ang.]: 0.6487299799919128
@>   Weight: 0.857143
@>   Energy [RT]: -3.24
@> Statistics for HIS157P-LYS112P:
@>   Average [Ang.]: 4.388020038604736
@>   Standard deviation [Ang.]: 1.0506110191345215
@>   Weight: 0.47619
@>   Energy [RT]: -2.14
@> Statistics for PHE138P-ARG58P:
@>   Average [Ang.]: 5.318399906158447
@>   Standard deviation [Ang.]: 0.24265700578689575
@>   Weight: 0.809524
@>   Energy [RT]: -4.51
@> Statistics for TYR87P-LYS112P:
@>   Average [Ang.]: 5.441559791564941
@>   Standard deviation [Ang.]: 0.25401198863983154
@>   Weight: 0.47619
@>   Energy [RT]: -2.64
@> Statistics for TRP39P-LYS6P:
@>   Average [Ang.]: 5.522061824798584
@>   Standard deviation [Ang.]: 0.31886300444602966
@>   Weight: 0.380952
@>   Energy [RT]: -3.12
@> Statistics for PHE85P-ARG75P:
@>   Average [Ang.]: 5.877999782562256
```

```
@>   Standard deviation [Ang.]: 0.06788399815559387
@>   Weight: 0.285714
@>   Energy [RT]: -4.51
```

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

```
@> Statistics for ARG101P-ASP98P:
@>   Average [Ang.]: 2.793931
@>   Standard deviation [Ang.]: 0.205527
@>   Weight: 1.52381
@>   Energy [RT]: -3.92
@> Statistics for HIS72P-ASN15P:
@>   Average [Ang.]: 2.989283
@>   Standard deviation [Ang.]: 0.270697
@>   Weight: 0.285714
@>   Energy [RT]: -3.05
@> Statistics for GLN143P-GLU139P:
@>   Average [Ang.]: 3.051633
@>   Standard deviation [Ang.]: 0.20753
@>   Weight: 1.285714
@>   Energy [RT]: -3.45
@> Statistics for HIS66P-GLU139P:
@>   Average [Ang.]: 2.900411
@>   Standard deviation [Ang.]: 0.169455
@>   Weight: 0.428571
@>   Energy [RT]: -3.15
@> Statistics for ARG40P-LYS6P:
@>   Average [Ang.]: 3.055475
@>   Standard deviation [Ang.]: 0.213814
@>   Weight: 0.380952
@>   Energy [RT]: -2.11
@> Statistics for ARG58P-ASP56P:
@>   Average [Ang.]: 2.827481
@>   Standard deviation [Ang.]: 0.171087
@>   Weight: 2.952381
@>   Energy [RT]: -3.92
@> Statistics for ALA45P-ARG75P:
@>   Average [Ang.]: 2.840721
@>   Standard deviation [Ang.]: 0.105565
@>   Weight: 0.904762
@>   Energy [RT]: -3.26
@> Statistics for ASN53P-GLU50P:
@>   Average [Ang.]: 2.980214
@>   Standard deviation [Ang.]: 0.147229
@>   Weight: 0.333333
@>   Energy [RT]: -2.43
@> Statistics for ALA74P-ASN53P:
@>   Average [Ang.]: 2.98522
@>   Standard deviation [Ang.]: 0.148331
@>   Weight: 0.952381
@>   Energy [RT]: -2.06
@> Statistics for ASP56P-ILE16P:
@>   Average [Ang.]: 3.085957
@>   Standard deviation [Ang.]: 0.21134
@>   Weight: 0.666667
@>   Energy [RT]: -3.46
@> Statistics for LYS110P-THR84P:
@>   Average [Ang.]: 2.774475
```

```
@>   Standard deviation [Ang.]: 0.080304
@>   Weight: 0.380952
@>   Energy [RT]: -1.64
@> Statistics for LEU116P-CYS90P:
@>   Average [Ang.]: 2.887425
@>   Standard deviation [Ang.]: 0.118768
@>   Weight: 0.952381
@>   Energy [RT]: -6.13
@> Statistics for SER103P-LEU99P:
@>   Average [Ang.]: 2.897324
@>   Standard deviation [Ang.]: 0.17182
@>   Weight: 1.380952
@>   Energy [RT]: -4.12
@> Statistics for ASN134P-ASP137P:
@>   Average [Ang.]: 2.917242
@>   Standard deviation [Ang.]: 0.160488
@>   Weight: 0.904762
@>   Energy [RT]: -2.5
@> Statistics for PHE152P-CYS148P:
@>   Average [Ang.]: 2.956784
@>   Standard deviation [Ang.]: 0.160039
@>   Weight: 0.904762
@>   Energy [RT]: -4.81
@> Statistics for ASN95P-ASP92P:
@>   Average [Ang.]: 3.061373
@>   Standard deviation [Ang.]: 0.215848
@>   Weight: 0.714286
@>   Energy [RT]: -2.5
@> Statistics for LYS6P-ASN38P:
@>   Average [Ang.]: 3.006786
@>   Standard deviation [Ang.]: 0.154497
@>   Weight: 0.333333
@>   Energy [RT]: -1.63
@> Statistics for ILE77P-ALA45P:
@>   Average [Ang.]: 2.819429
@>   Standard deviation [Ang.]: 0.092538
@>   Weight: 0.666667
@>   Energy [RT]: -4.45
@> Statistics for LEU99P-ASN95P:
@>   Average [Ang.]: 3.027242
@>   Standard deviation [Ang.]: 0.19744
@>   Weight: 0.904762
@>   Energy [RT]: -3.94
..
..
```

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
@>   Energy [RT]: -3.92
@> Statistics for HIS72P-ASN15P:
@>   Average [Ang.]: 2.989283
@>   Standard deviation [Ang.]: 0.270697
@>   Weight: 0.285714
@>   Energy [RT]: -3.05
@> Statistics for HIS66P-GLU139P:
@>   Average [Ang.]: 2.900411
@>   Standard deviation [Ang.]: 0.169455
@>   Weight: 0.428571
@>   Energy [RT]: -3.15
@> Statistics for ARG40P-LYS6P:
@>   Average [Ang.]: 3.055475
@>   Standard deviation [Ang.]: 0.213814
@>   Weight: 0.380952
@>   Energy [RT]: -2.11
@> Statistics for ARG58P-ASP56P:
@>   Average [Ang.]: 2.827481
@>   Standard deviation [Ang.]: 0.171087
@>   Weight: 2.952381
@>   Energy [RT]: -3.92
@> Statistics for ALA45P-ARG75P:
@>   Average [Ang.]: 2.840721
@>   Standard deviation [Ang.]: 0.105565
@>   Weight: 0.904762
@>   Energy [RT]: -3.26
@> Statistics for ASN53P-GLU50P:
@>   Average [Ang.]: 2.980214
@>   Standard deviation [Ang.]: 0.147229
@>   Weight: 0.333333
@>   Energy [RT]: -2.43
@> Statistics for ALA74P-ASN53P:
@>   Average [Ang.]: 2.98522
@>   Standard deviation [Ang.]: 0.148331
@>   Weight: 0.952381
@>   Energy [RT]: -2.06
..
..
```

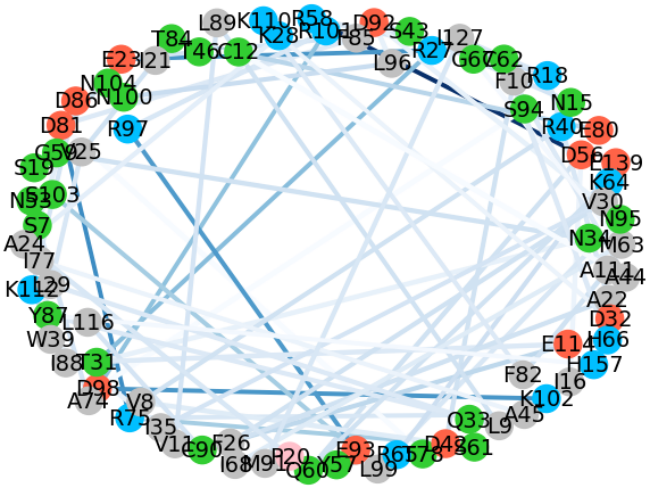
We can also use the `showInteractionsHist()` function to display the results as a bar plot (`clip` define how many pair we would like to display).

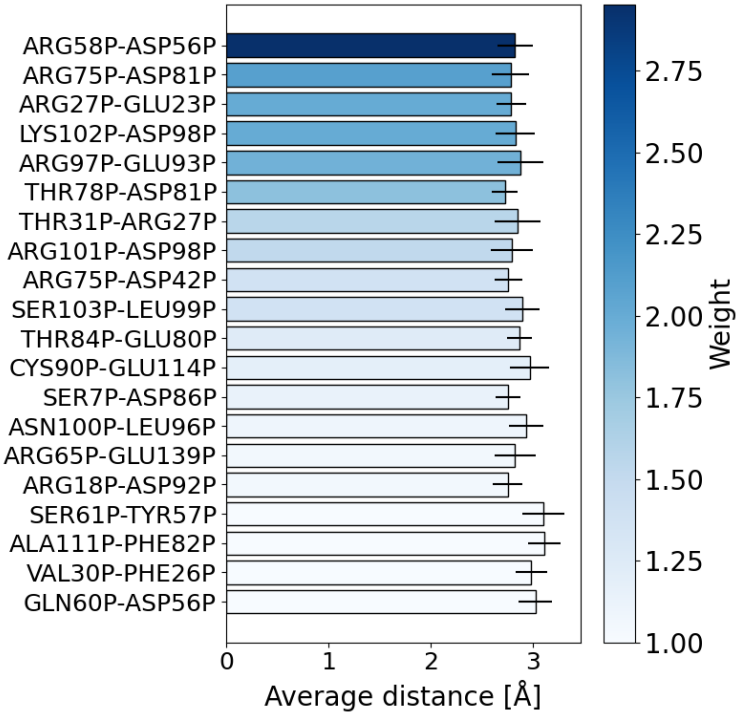
```
In [39]: showInteractionsHist(statistics, clip=20)
```

7.5 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:




ARG58P-ASP56P
ARG75P-ASP81P
ARG27P-GLU23P
LYS102P-ASP98P
ARG97P-GLU93P
THR78P-ASP81P
THR31P-ARG27P
ARG101P-ASP98P
ARG75P-ASP42P
SER103P-LEU99P
THR84P-GLU80P
CYS90P-GLU114P
SER7P-ASP86P
ASN100P-LEU96P
ARG65P-GLU139P
ARG18P-ASP92P
SER61P-TYR57P
ALA111P-PHE82P
VAL30P-PHE26P
GLN60P-ASP56P
0
1
2
3
Average distance [Å]
2.75
2.50
2.25
2.00
1.75
1.50
1.25
1.00
Weight

```
In [40]: frame0 = dcd.getFrame(0)

In [41]: at0 = frame0.getAtoms()

In [42]: 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 [43]: frame18 = dcd.getFrame(18)

In [44]: at18 = frame18.getAtoms()

In [45]: 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 [46]: 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:

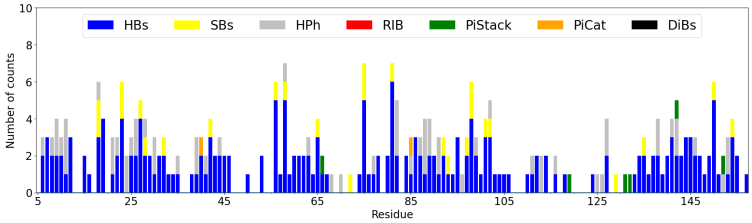
```
In [47]: interactions0 = Interactions()
```

```
In [48]: interactions0.calcProteinInteractions(at0)

In [49]: matrix0 = interactions0.buildInteractionMatrix()
```

```
In [50]: interactions0.showCumulativeInteractionTypes()
```

```
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
```




```
In [51]: interactions18 = Interactions()

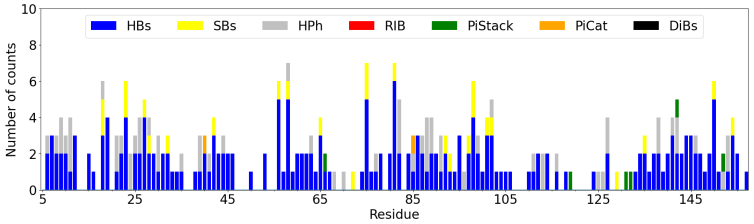
In [52]: interactions18.calcProteinInteractions(at18)

In [53]: 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 [54]: interactions18.showCumulativeInteractionTypes()
```

```
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
@> Calculating interaction matrix
```



7.6 Parse previously saved data

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

```
In [55]: interactionsTrajectory2 = InteractionsTrajectory('5kqm_import')

In [56]: 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 [57]: interactionsTrajectory2.getHydrophohic()
```

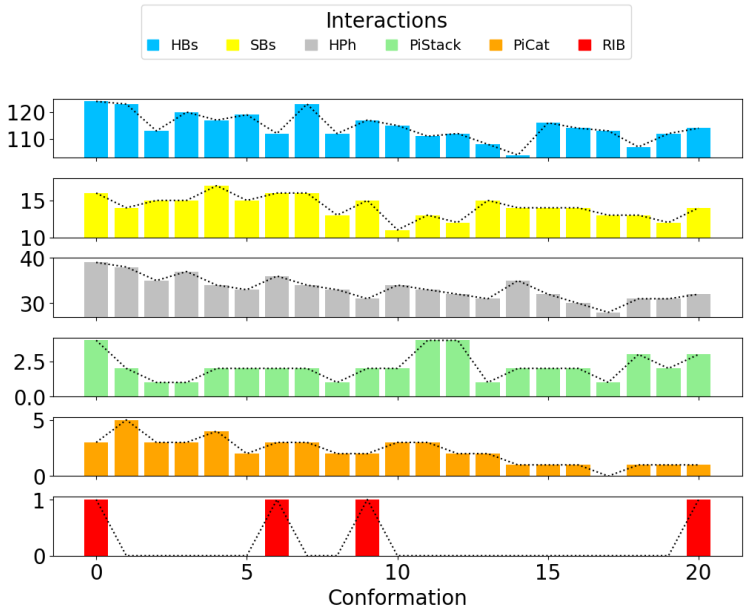
```
[[['ALA156', 'CB_2401', 'P', 'TYR87', 'OH_1286', 'P', 3.0459, 21.959],
  ['ALA24', 'CB_298', 'P', 'MET63', 'CE_894', 'P', 3.3105, 5.1584],
  ['ILE68', 'CG2_976', 'P', 'MET63', 'CE_894', 'P', 3.3306, 52.4165],
  ['TYR142', 'CZ_2171', 'P', 'VAL146', 'CG2_2235', 'P', 3.4815, 49.7427],
  ['PHE10', 'CD1_92', '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 [58]: calcStatisticsInteractions(interactionsTrajectory2.getHydrogenBonds())
```

```
@> Statistics for ARG101P-ASP98P:
@>   Average [Ang.]: 2.793931
@>   Standard deviation [Ang.]: 0.205527
@>   Weight: 1.52381
@>   Energy [RT]: -3.92
@> Statistics for HIS72P-ASN15P:
@>   Average [Ang.]: 2.989283
@>   Standard deviation [Ang.]: 0.270697
@>   Weight: 0.285714
@>   Energy [RT]: -3.05
@> Statistics for GLN143P-GLU139P:
@>   Average [Ang.]: 3.051633
@>   Standard deviation [Ang.]: 0.20753
@>   Weight: 1.285714
@>   Energy [RT]: -3.45
@> Statistics for HIS66P-GLU139P:
@>   Average [Ang.]: 2.900411
@>   Standard deviation [Ang.]: 0.169455
@>   Weight: 0.428571
@>   Energy [RT]: -3.15
@> Statistics for ARG40P-LYS6P:
@>   Average [Ang.]: 3.055475
@>   Standard deviation [Ang.]: 0.213814
@>   Weight: 0.380952
@>   Energy [RT]: -2.11
@> Statistics for ARG58P-ASP56P:
@>   Average [Ang.]: 2.827481
@>   Standard deviation [Ang.]: 0.171087
@>   Weight: 2.952381
@>   Energy [RT]: -3.92
..
..
```

```
In [59]: interactionsTrajectory2.getTimeInteractions()
```


Interactions
HBs
SBs
HPh
PiStack
PiCat
RIB
120
110
15
10
40
30
2.5
0.0
5
0
1
0
0
5
10
15
20
Conformation

CHAPTER

EIGHT

SIGNATURE INTERACTIONS OF ENSEMBLES

We have developed a pipeline that leverages BLAST, Dali, or Foldseek search to identify and download homologs for a particular PDB structure. The identified structures are prepared for InSty analysis by applying the following steps: (i) download PDB, (ii) extract particular chains, (iii) add hydrogens/side chains, (iv) perform structural alignment, (v) create a folder with prepared structures in it.

As an example, we will use Aurora kinase A structure (PDB code: **1OL5**).

8.1 BLAST approach

We will use the PDB code and chain ID to access information from the BLAST server. Additionally, we can also define many different types of parameters. Here, we will define sequence identity (`seqid`) and the method to add missing hydrogen bonds and side chains (`fixer`; it can be PDBFixer or Openbabel). We can also define a name for a folder in which all the downloaded files will be uploaded (`folder_name`).

To download homologs, add missing hydrogens and align structures, we will use the `runBLAST()` function:

```
In [1]: PDBcode = '1ol5'

In [2]: runBLAST(PDBcode, 'A', seqid=70, fixer='openbabel', folder_name='struc_homologs_BLAST')
```

```
@> PDB file is found in working directory (1ol5.pdb).
@> 2607 atoms and 1 coordinate set(s) were parsed in 0.03s.
@> Blast searching NCBI PDB database for "SKKRQ..."
@> Blast search completed in 46.3s.
@> Separating chains and saving into PDB file
@> PDB code 1muo and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 1muo downloaded (1muo.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 2029 atoms and 1 coordinate set(s) were parsed in 0.07s.
@> PDB code 2j4z and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 2j4z downloaded (2j4z.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 4626 atoms and 1 coordinate set(s) were parsed in 0.14s.
@> PDB code 7o2v and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 7o2v downloaded (7o2v.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 2265 atoms and 1 coordinate set(s) were parsed in 0.10s.
@> PDB code 6c83 and chain A
```

```
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 6c83 downloaded (6c83.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 4937 atoms and 1 coordinate set(s) were parsed in 0.16s.
@> PDB code 6cpe and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 6cpe downloaded (6cpe.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 4024 atoms and 1 coordinate set(s) were parsed in 0.13s.
@> PDB code 6cpf and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 6cpf downloaded (6cpf.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 4100 atoms and 1 coordinate set(s) were parsed in 0.13s.
@> PDB code 6cpg and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 6cpg downloaded (6cpg.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 9962 atoms and 1 coordinate set(s) were parsed in 0.20s.
@> PDB code 8sso and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 8sso downloaded (8sso.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 6151 atoms and 1 coordinate set(s) were parsed in 0.18s.
@> PDB code 2xng and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 2xng downloaded (2xng.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 2001 atoms and 1 coordinate set(s) were parsed in 0.07s.
@> PDB code 4b0g and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 4b0g downloaded (4b0g.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 2065 atoms and 1 coordinate set(s) were parsed in 0.07s.
@> PDB code 8ssp and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 8ssp downloaded (8ssp.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 3066 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> PDB code 2x6d and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 2x6d downloaded (2x6d.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 2144 atoms and 1 coordinate set(s) were parsed in 0.08s.
@> PDB code 2x6e and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 2x6e downloaded (2x6e.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
```

```
@> 2007 atoms and 1 coordinate set(s) were parsed in 0.06s.
@> PDB code 4byi and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 4byi downloaded (4byi.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 2049 atoms and 1 coordinate set(s) were parsed in 0.09s.
@> PDB code 4byj and chain A
..
..
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 5k3y downloaded (5k3y.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 5831 atoms and 1 coordinate set(s) were parsed in 0.19s.
@> Adding hydrogens to the structures..
@> Hydrogens were added to the structure. New structure is saved as addH_1muoA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_2j4zA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_7o2vA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_6c83A.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_6cpeA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_6cpfA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_6cpgA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_8ssoA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_2xngA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_4b0gA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_8sspA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_2x6dA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_2x6eA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_4byiA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_4byjA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_4zs0A.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_4ztqA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_4ztrA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_4ztsA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_5oneA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_6graA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_6z4yA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_7ayhA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_7ayiA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_5zanA.pdb.
..
..
@> Hydrogens were added to the structure. New structure is saved as addH_2vgoA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_2vgpA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_3ztxA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_2vrxA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_4c2vA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_4c2wA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_6gr8A.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_6gr9A.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_2bfyA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_5eykA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_5k3yA.pdb.
@> 209 PDBs were parsed in 8.49s.
@> Aligning the structures..
@> addH_2j4zA
@> Checking AtomGroup addH_2j4zA: 1 chains are identified
```

```
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_2j4zA (len=263) and Chain A from addH_1muoA (len=251):
@>   Match: 251 residues match with 100% sequence identity and 95% overlap.
@> Aligning the structures..
@> addH_7o2vA
@> Checking AtomGroup addH_7o2vA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_7o2vA (len=264) and Chain A from addH_1muoA (len=251):
@>   Match: 250 residues match with 100% sequence identity and 95% overlap.
@> Aligning the structures..
@> addH_6c83A
@> Checking AtomGroup addH_6c83A: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_6c83A (len=248) and Chain A from addH_1muoA (len=251):
@>   Match: 246 residues match with 99% sequence identity and 98% overlap.
@> Aligning the structures..
@> addH_6cpeA
@> Checking AtomGroup addH_6cpeA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_6cpeA (len=256) and Chain A from addH_1muoA (len=251):
@>   Match: 248 residues match with 99% sequence identity and 97% overlap.
@> Aligning the structures..
@> addH_6cpfA
@> Checking AtomGroup addH_6cpfA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_6cpfA (len=259) and Chain A from addH_1muoA (len=251):
@>   Match: 249 residues match with 99% sequence identity and 96% overlap.
@> Aligning the structures..
@> addH_6cpgA
@> Checking AtomGroup addH_6cpgA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_6cpgA (len=249) and Chain A from addH_1muoA (len=251):
@>   Match: 248 residues match with 100% sequence identity and 99% overlap.
@> Aligning the structures..
@> addH_8ssoA
@> Checking AtomGroup addH_8ssoA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_8ssoA (len=256) and Chain A from addH_1muoA (len=251):
@>   Match: 251 residues match with 100% sequence identity and 98% overlap.
@> Aligning the structures..
@> addH_2xngA
@> Checking AtomGroup addH_2xngA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_2xngA (len=253) and Chain A from addH_1muoA (len=251):
@>   Match: 248 residues match with 99% sequence identity and 98% overlap.
@> Aligning the structures..
@> addH_4b0gA
@> Checking AtomGroup addH_4b0gA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
```

```
@>   Comparing Chain A from addH_4b0gA (len=247) and Chain A from addH_1muoA (len=251):
@>   Match: 241 residues match with 98% sequence identity and 96% overlap.
@> Aligning the structures..
@> addH_8sspA
@> Checking AtomGroup addH_8sspA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_8sspA (len=264) and Chain A from addH_1muoA (len=251):
@>   Match: 251 residues match with 100% sequence identity and 95% overlap.
@> Aligning the structures..
@> addH_2x6dA
@> Checking AtomGroup addH_2x6dA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_2x6dA (len=255) and Chain A from addH_1muoA (len=251):
@>   Match: 246 residues match with 98% sequence identity and 96% overlap.
@> Aligning the structures..
@> addH_2x6eA
@> Checking AtomGroup addH_2x6eA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_2x6eA (len=249) and Chain A from addH_1muoA (len=251):
@>   Match: 245 residues match with 98% sequence identity and 98% overlap.
@> Aligning the structures..
@> addH_4byiA
@> Checking AtomGroup addH_4byiA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_4byiA (len=254) and Chain A from addH_1muoA (len=251):
@>   Match: 249 residues match with 99% sequence identity and 98% overlap.
@> Aligning the structures..
@> addH_4byjA
@> Checking AtomGroup addH_4byjA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_4byjA (len=246) and Chain A from addH_1muoA (len=251):
@>   Match: 244 residues match with 99% sequence identity and 97% overlap.
@> Aligning the structures..
@> addH_4zs0A
@> Checking AtomGroup addH_4zs0A: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_4zs0A (len=257) and Chain A from addH_1muoA (len=251):
@>   Match: 248 residues match with 99% sequence identity and 96% overlap.
..
..
@> Aligning the structures..
@> addH_5eykA
@> Checking AtomGroup addH_5eykA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_5eykA (len=264) and Chain A from addH_1muoA (len=251):
@>   Failed to match chains (seqid=5%, overlap=81%).
@> Trying to match chains based on local sequence alignment:
@>  Comparing Chain A from addH_5eykA (len=264) and Chain A from addH_1muoA (len=251):
@>   Match: 246 residues match with 70% sequence identity and 93% overlap.
@> Aligning the structures..
@> addH_5k3yA
```

```
@> Checking AtomGroup addH_5k3yA: 1 chains are identified
@> Checking AtomGroup addH_1muoA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_5k3yA (len=268) and Chain A from addH_1muoA (len=251):
@>   Failed to match chains (seqid=5%, overlap=81%).
@> Trying to match chains based on local sequence alignment:
@>  Comparing Chain A from addH_5k3yA (len=268) and Chain A from addH_1muoA (len=251):
@>   Match: 246 residues match with 71% sequence identity and 92% overlap.
```

To compute all types of interactions for each homolog, we use the `calcSignatureInteractions()` function, and we are providing the name of the folder with the structures.

This function will create additional files with the prefix `'INT_'+type_of_interactions` for each file. In such a file besides the protein structure, we will have dummy atoms that will correspond to the interactions. The dummy atoms will be inserted exactly between the residue-residue pair which is interacting. We are computing seven types of non-covalent interactions (hydrogen bonds - `HBs`, salt bridges - `SBs`, repulsive ionic bonding - `RIB`, pi-cation - `PiCat`, pi-stacking - `PiStack`, hydrophobic interactions - `HPh`, and disulfide bonds - `DiBs`).

```
In [3]: calcSignatureInteractions('struc_homologs_BLAST')
```

```
@> struc_homologs_BLAST/align__addH_5i8kA.pdb
@> 4385 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)    <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     LEU178    A         N_868  <--->     VAL174    A         O_808     2.8    25.5
@>     GLU321    A        N_3203  <--->     VAL317    A        O_3141     2.8    27.8
@>     VAL324    A        N_3257  <--->     TYR320    A        O_3187     2.9    37.4
@>     LEU208    A        N_1397  <--->     LYS162    A         O_609     2.9    31.8
@>     ILE360    A        N_3839  <--->     ALA356    A        O_3779     2.9    19.9
@>     LYS224    A        N_1666  <--->     ARG220    A        O_1596     2.9    39.0
@>     LEU263    A        N_2315  <--->     LYS271    A        O_2427     2.9    34.6
@>     LEU318    A        N_3152  <--->     SER314    A        O_3104     2.9    35.1
@>     GLY173    A         N_796  <--->     GLU170    A         O_754     3.0    38.1
@>     LEU149    A         N_377  <--->     ARG137    A         O_189     3.0    28.6
@>     ALA243    A        N_1978  <--->     GLU239    A        O_1925     3.0    23.2
@>     ILE253    A        N_2140  <--->     SER278    A        O_2541     3.0    23.1
@>     TYR236    A        N_1866  <--->     ARG232    A        O_1809     3.0     7.4
@>     SER314    A        N_3099  <--->     VAL310    A        O_3033     3.0    30.1
@>     ARG220    A        N_1591  <--->     THR217    A      OG1_1548     3.0    17.6
@>     ILE193    A        N_1133  <--->     HIS190    A        O_1093     3.0    13.9
@>     VAL317    A        N_3136  <--->     TRP313    A        O_3080     3.0    34.9
@>     SER342    A        N_3556  <--->     TYR338    A        O_3475     3.0    25.6
@>     THR337    A        N_3456  <--->     THR333    A        O_3394     3.0    24.4
@>     TYR320    A        N_3182  <--->     GLY316    A        O_3135     3.1    39.9
@>     LEU169    A         N_730  <--->     PHE165    A         O_666     3.1    35.0
@>     LEU315    A        N_3110  <--->     ASP311    A        O_3049     3.1    22.9
@>     HIS187    A        N_1028  <--->     ILE184    A         O_986     3.1    38.9
@>     ARG362    A        N_3869  <--->     ASP358    A        O_3813     3.1    23.5
@>     PHE133    A         N_123  <--->     LEU130    A          O_82     3.1     3.3
@>     HIS380    A        N_4189  <--->     VAL377    A        O_4144     3.1    34.9
@>     LEU363    A        N_3893  <--->     LEU359    A        O_3825     3.1    39.5
@>     GLY316    A        N_3129  <--->     LEU312    A        O_3061     3.1    36.0
@>     LYS339    A        N_3491  <--->     GLN335    A        O_3429     3.1    15.1
@>     ILE184    A         N_981  <--->     ARG180    A         O_916     3.1    16.3
@>     LEU359    A        N_3820  <--->     GLY355    A        O_3773     3.1    37.9
@>     ARG179    A         N_887  <--->     GLU175    A         O_824     3.2     4.7
@>     LEU262    A        N_2296  <--->     PRO259    A        O_2257     3.2    25.9
@>     VAL352    A        N_3722  <--->     PRO349    A        O_3680     3.2    26.7
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@>     VAL377    A        N_4139  <--->     MET373    A        O_4069     3.2    15.7
@>     GLU183    A         N_966  <--->     ARG179    A         O_892     3.2     6.3
@>     TYR219    A        N_1570  <--->     PRO259    A        O_2257     3.2    39.1
@>     LYS309    A       NZ_3024  <--->     PRO372    A        O_4054     3.2    38.5
@>     ALA172    A         N_786  <--->     GLN168    A         O_718     3.2     6.7
@>     LEU323    A        N_3238  <--->     CYS319    A        O_3176     3.2    13.8
@>     GLU221    A        N_1615  <--->     THR217    A        O_1545     3.2    24.1
@>     ALA241    A        N_1954  <--->     THR238    A        O_1911     3.3    37.2
@>     GLU336    A        N_3441  <--->     THR333    A        O_3394     3.3    13.4
@>     ILE301    A        N_2880  <--->     PRO297    A        O_2824     3.3    24.6
@>     HIS248    A        N_2050  <--->     SER245    A        O_2012     3.4    38.4
@>     ARG205    A       NE_1351  <--->     ASP202    A      OD2_1311     3.4    29.3
@>     SER245    A        N_2007  <--->     ASN242    A        O_1969     3.4    31.2
@>     THR333    A        N_3389  <--->     GLU336    A      OE1_3454     3.4    29.4
@>     GLY140    A         N_241  <--->     VAL147    A         O_345     3.4    25.0
@>     LEU225    A        N_1688  <--->     LEU222    A        O_1635     3.5    35.1
@>     LYS166    A         NZ_699  <--->     ALA203    A        O_1317     3.5    31.4
@>     ASN386    A      ND2_4298  <--->     TRP382    A      NE1_4233     3.5    40.0
@>     GLY145    A         N_319  <--->     GLY142    A         O_276     3.5    32.9
@>     LYS250    A        N_2078  <--->     TYR246    A        O_2023     3.5    14.1
@> Number of detected hydrogen bonds: 54.
@> Creating file with dummy atoms
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@> 4154 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     PHE241    A        N_1708  <--->     PHE335    A        O_3061     2.8    39.0
@>     LEU162    A         N_337  <--->     ARG150    A         O_149     2.8    30.9
@>     LEU172    A         N_518  <--->     ALA163    A         O_361     2.9    30.2
@>     LYS179    A         N_643  <--->     THR217    A        O_1293     2.9    21.4
@>     ASP269    A        N_2168  <--->     ASP287    A      OD2_2456     2.9    28.9
@>     PHE335    A        N_3056  <--->     LEU331    A        O_2995     2.9    34.2
@>     ILE222    A        N_1382  <--->     GLY211    A        O_1207     2.9    31.4
@>     ARG384    A       NE_3875  <--->     LYS378    A        O_3774     2.9    28.1
@>     ARG208    A        N_1137  <--->     GLU224    A      OE2_1434     2.9    11.0
@>     GLN236    A        N_1615  <--->     TYR232    A        O_1541     2.9     8.0
@>     GLN190    A       NE2_831  <--->     GLU194    A       OE2_915     2.9    28.4
@>     LEU238    A        N_1654  <--->     GLU234    A        O_1586     2.9    25.0
@>     CYS260    A        N_2007  <--->     ALA256    A        O_1951     2.9    34.8
@>     ASP371    A        N_3646  <--->     GLU367    A        O_3595     3.0    35.9
@>     ARG356    A        N_3405  <--->     ARG352    A        O_3332     3.0    36.5
@>     GLU165    A         N_390  <--->     PHE170    A         O_484     3.0    39.4
@>     GLU196    A         N_932  <--->     ARG192    A         O_858     3.0    20.9
@>     ILE373    A        N_3677  <--->     ALA369    A        O_3617     3.0    37.6
@>     LYS263    A        N_2046  <--->     TYR259    A        O_1991     3.0    17.9
@>     ARG352    A        N_3327  <--->     GLN348    A        O_3265     3.0     2.1
@>     VAL330    A        N_2974  <--->     TRP326    A        O_2918     3.0    37.0
@>     ARG233    A        N_1557  <--->     THR230    A      OG1_1514     3.0    21.3
@>     TYR308    A        N_2618  <--->     THR305    A        O_2578     3.0     3.8
@>     ALA185    A         N_752  <--->     GLN181    A         O_684     3.0    35.9
@>     ARG192    A         N_853  <--->     GLU188    A         O_790     3.0    36.0
@>     HIS261    A        N_2018  <--->     LEU257    A        O_1961     3.1    32.6
@>     ASP324    A        N_2882  <--->     ASP320    A        O_2822     3.1     2.2
@>     GLU252    A        N_1888  <--->     THR248    A        O_1825     3.1    17.2
@>     SER262    A        N_2035  <--->     SER258    A        O_1980     3.1    19.0
@>     LEU182    A         N_696  <--->     PHE178    A         O_628     3.1    13.4
@>     GLY158    A         N_279  <--->     GLY155    A         O_236     3.1    33.6
@>     ARG375    A        N_3707  <--->     ASP371    A        O_3651     3.1    11.7
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@>     GLU194    A         N_901  <--->     GLN190    A         O_822     3.1    20.1
@>     VAL323    A        N_2866  <--->     ASP320    A      OD1_2827     3.1    12.3
@>     TYR333    A        N_3020  <--->     GLY329    A        O_2973     3.1    36.7
@>     GLU349    A        N_3277  <--->     THR346    A      OG1_3233     3.1    22.2
@>     LEU325    A        N_2894  <--->     GLU321    A        O_2834     3.1    15.2
@>     ARG193    A         N_877  <--->     HIS189    A         O_805     3.1    33.8
@>     SER327    A        N_2937  <--->     VAL323    A        O_2871     3.1    22.3
@>     HIS393    A        N_4011  <--->     VAL390    A        O_3966     3.2    26.4
@>     LEU372    A        N_3658  <--->     GLY368    A        O_3611     3.2    26.4
@>     THR350    A        N_3292  <--->     THR346    A        O_3230     3.2    18.0
@>     ILE197    A         N_947  <--->     ARG193    A         O_882     3.2    33.7
@>     GLY329    A        N_2967  <--->     LEU325    A        O_2899     3.2    22.1
@>     LEU376    A        N_3731  <--->     LEU372    A        O_3663     3.2    39.7
@>     GLY186    A         N_762  <--->     GLU183    A         O_720     3.2    16.4
@>     VAL187    A         N_769  <--->     LEU182    A         O_701     3.2     9.9
@>     TYR232    A        N_1536  <--->     PRO272    A        O_2225     3.2    26.8
@>     LEU336    A        N_3076  <--->     CYS332    A        O_3014     3.2    32.0
@>     GLU389    A        N_3946  <--->     THR386    A      OG1_3911     3.2    35.4
@>     ASN399    A        N_4117  <--->     ILE396    A        O_4071     3.3    27.4
@>     GLU392    A        N_3996  <--->     ALA388    A        O_3941     3.4    17.0
@>     ILE314    A        N_2718  <--->     PRO310    A        O_2662     3.4    20.0
@>     LYS179    A        NZ_661  <--->     HIS214    A      ND1_1259     3.5    35.5
@>     ARG384    A      NH1_3878  <--->     HIS379    A        O_3796     3.5    11.1
@> Number of detected hydrogen bonds: 55.
@> Creating file with dummy atoms
@> struc_homologs_BLAST/align__addH_2x6dA.pdb
@> 4202 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     PHE322    A        N_3096  <--->     LEU318    A        O_3035     2.8    15.1
@>     LEU240    A        N_1880  <--->     TYR236    A        O_1816     2.8    33.3
@>     SER361    A        N_3736  <--->     ARG357    A        O_3667     2.9    30.2
@>     SER342    A        N_3434  <--->     TYR338    A        O_3353     2.9    39.1
@>     ARG343    A        N_3445  <--->     LYS339    A        O_3374     2.9    38.2
@>     GLN223    A        N_1594  <--->     TYR219    A        O_1520     2.9     7.0
@>     THR238    A        N_1851  <--->     ALA234    A        O_1792     2.9    38.2
@>     THR235    A        N_1797  <--->     GLN231    A        O_1737     2.9     9.8
@>     CYS319    A        N_3049  <--->     LEU315    A        O_2993     2.9    37.4
@>     LEU315    A        N_2988  <--->     ASP311    A        O_2927     2.9     9.6
@>     ASN242    A        N_1909  <--->     THR238    A        O_1856     3.0    39.2
@>     ARG362    A        N_3747  <--->     ASP358    A        O_3691     3.0    28.4
@>     TYR246    A        N_1963  <--->     ASN242    A        O_1914     3.0    36.6
@>     SER283    A        N_2549  <--->     HIS306    A        O_2845     3.0    34.3
@>     CYS247    A        N_1984  <--->     ALA243    A        O_1928     3.0    12.8
@>     TYR320    A        N_3060  <--->     GLY316    A        O_3013     3.0    35.7
@>     TYR338    A        N_3348  <--->     TYR334    A        O_3286     3.0    34.3
@>     SER186    A         N_962  <--->     VAL182    A         O_900     3.0    28.2
@>     GLU379    A        N_4052  <--->     ARG375    A        O_3983     3.0    32.3
@>     VAL344    A        N_3469  <--->     ILE341    A        O_3420     3.0    37.7
@>     ILE209    A        N_1361  <--->     GLY198    A        O_1186     3.0    29.7
@>     HIS248    A      NE2_2010  <--->     ASP311    A      OD2_2933     3.1    23.7
@>     ASP256    A        N_2145  <--->     HIS254    A      ND1_2114     3.1    36.7
@>     LYS271    A       NZ_2385  <--->     PRO191    A        O_1054     3.1    32.9
@>     VAL377    A        N_4017  <--->     MET373    A        O_3947     3.1    27.4
@>     LEU323    A        N_3116  <--->     CYS319    A        O_3054     3.1    16.5
@>     HIS380    A        N_4067  <--->     VAL377    A        O_4022     3.2    21.1
@>     THR233    A        N_1773  <--->     ASP229    A        O_1710     3.2    32.3
@>     GLU336    A        N_3319  <--->     THR333    A        O_3272     3.2    26.9
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@>     HIS306    A        N_2840  <--->     SER283    A        O_2554     3.2    18.0
@>     TRP313    A        N_2953  <--->     LYS309    A        O_2889     3.2    31.5
@>     ALA356    A        N_3652  <--->     THR353    A      OG1_3624     3.2    16.9
@>     ARG371    A        N_3904  <--->     PRO368    A        O_3866     3.2    19.6
@>     VAL182    A         N_895  <--->     ARG179    A         O_837     3.2    31.6
@>     ARG371    A      NH1_3922  <--->     HIS366    A        O_3836     3.2    39.7
@>     SER314    A        N_2977  <--->     VAL310    A        O_2911     3.3    19.9
@>     GLU134    A         N_143  <--->     ARG151    A         O_411     3.3    17.4
@>     LYS224    A       NZ_1629  <--->     GLU221    A      OE1_1573     3.3    25.2
@>     LYS250    A        N_2023  <--->     TYR246    A        O_1968     3.3    38.1
@>     ARG179    A         N_832  <--->     GLU175    A         O_769     3.3    25.3
@>     LEU359    A        N_3698  <--->     GLY355    A        O_3651     3.3     9.3
@>     LEU169    A         N_730  <--->     PHE165    A         O_666     3.4     6.5
@>     TYR219    A        N_1515  <--->     PRO259    A        O_2202     3.4    26.8
@>     THR384    A        N_4141  <--->     PRO381    A        O_4088     3.4    39.9
@>     GLY316    A        N_3007  <--->     LEU312    A        O_2939     3.4    18.4
@>     LYS339    A        N_3369  <--->     GLN335    A        O_3307     3.4    18.9
@>     HIS254    A      ND1_2114  <--->     ILE257    A        N_2157     3.4    35.9
@>     LEU270    A        N_2348  <--->     GLU239    A      OE1_1878     3.4    36.6
@>     LYS224    A        N_1611  <--->     GLU221    A        O_1565     3.4    32.2
@>     LYS271    A       NZ_2385  <--->     GLU211    A      OE2_1413     3.4    35.6
@>     ARG304    A      NH2_2820  <--->     HIS366    A      NE2_3847     3.4    27.2
@>     HIS248    A        N_1995  <--->     SER245    A        O_1957     3.5    38.5
@>     VAL324    A        N_3135  <--->     GLU321    A        O_3086     3.5    32.7
@>     PHE157    A         N_517  <--->     GLU152    A         O_435     3.5    33.7
@>     LEU378    A        N_4033  <--->     ARG375    A        O_3983     3.5    37.4
@> Number of detected hydrogen bonds: 55.
@> Creating file with dummy atoms
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@> 4141 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     LEU243    A        N_1964  <--->     LEU239    A        O_1916     2.7    38.9
@>     GLN369    A        N_3804  <--->     ASN366    A        O_3770     2.8    29.7
@>     LEU221    A        N_1606  <--->     VAL217    A        O_1535     2.9    32.6
@>     ILE208    A        N_1392  <--->     GLY197    A        O_1217     2.9    16.0
@>     TRP381    A      NE1_4028  <--->     GLU229    A      OE2_1762     2.9    33.1
@>     ARG194    A        N_1147  <--->     GLU210    A      OE2_1444     2.9    40.0
@>     VAL217    A        N_1530  <--->     LEU261    A        O_2277     2.9    11.6
@>     TYR337    A        N_3265  <--->     TYR333    A        O_3203     2.9    33.3
@>     ALA233    A        N_1818  <--->     GLU229    A        O_1753     2.9    39.6
@>     LYS338    A        N_3286  <--->     GLN334    A        O_3224     3.0    25.4
@>     ILE183    A         N_957  <--->     ARG179    A         O_892     3.0    25.3
@>     GLU180    A         N_911  <--->     GLN176    A         O_832     3.0    14.5
@>     VAL251    A        N_2100  <--->     CYS246    A        O_2020     3.0    13.1
@>     ARG356    A        N_3579  <--->     THR352    A        O_3538     3.0    20.1
@>     ALA149    A         N_372  <--->     LEU158    A         O_537     3.0    38.4
@>     SER313    A        N_2894  <--->     VAL309    A        O_2828     3.0    38.0
@>     ARG342    A        N_3362  <--->     LYS338    A        O_3291     3.0    22.7
@>     ILE340    A        N_3332  <--->     THR336    A        O_3256     3.0    31.2
@>     CYS318    A        N_2966  <--->     LEU314    A        O_2910     3.0    23.8
@>     LEU158    A         N_532  <--->     ALA149    A         O_377     3.0    33.9
@>     LEU168    A         N_706  <--->     PHE164    A         O_642     3.0    17.4
@>     ALA384    A        N_4072  <--->     PRO380    A        O_4005     3.1    16.4
@>     LYS161    A         N_580  <--->     LEU207    A        O_1378     3.1    37.4
@>     SER341    A        N_3351  <--->     TYR337    A        O_3270     3.1    21.0
@>     ARG219    A        N_1567  <--->     THR216    A      OG1_1524     3.1    23.9
@>     LEU239    A        N_1911  <--->     TYR235    A        O_1847     3.1    29.2
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@>     VAL316    A        N_2931  <--->     TRP312    A        O_2875     3.1    33.5
@>     CYS246    A        N_2015  <--->     ALA242    A        O_1959     3.1    33.9
@>     THR232    A        N_1804  <--->     ASP228    A        O_1741     3.1    18.4
@>     LEU362    A        N_3688  <--->     LEU358    A        O_3620     3.1    37.1
@>     ILE359    A        N_3634  <--->     ALA355    A        O_3574     3.1    28.2
@>     SER387    A        N_4107  <--->     THR234    A      OG1_1836     3.1    23.1
@>     HIS379    A        N_3984  <--->     VAL376    A        O_3939     3.1     7.8
@>     LEU224    A        N_1664  <--->     GLU220    A        O_1596     3.2     3.5
@>     THR336    A        N_3251  <--->     THR332    A        O_3189     3.2    12.0
@>     GLU238    A        N_1896  <--->     THR234    A        O_1833     3.2    18.5
@>     ARG361    A        N_3664  <--->     ASP357    A        O_3608     3.2     8.1
@>     ASN241    A        N_1940  <--->     THR237    A        O_1887     3.2    20.2
@>     ASN260    A      ND2_2269  <--->     ASP255    A      OD1_2186     3.2    33.1
@>     GLY315    A        N_2924  <--->     LEU311    A        O_2856     3.2    28.2
@>     LEU358    A        N_3615  <--->     GLY354    A        O_3568     3.2    27.7
@>     TYR319    A        N_2977  <--->     GLY315    A        O_2930     3.2    17.1
@>     SER248    A        N_2043  <--->     SER244    A        O_1988     3.2    15.8
@>     LEU322    A        N_3033  <--->     CYS318    A        O_2971     3.2    27.9
@>     THR237    A        N_1882  <--->     ALA233    A        O_1823     3.2    24.3
@>     LEU214    A        N_1490  <--->     LEU263    A        O_2315     3.2    33.9
@>     VAL146    A         N_316  <--->     GLY139    A         O_223     3.3    31.4
@>     ASN385    A        N_4082  <--->     TRP381    A        O_4020     3.3    37.2
@>     GLU378    A        N_3969  <--->     ARG374    A        O_3900     3.3    27.3
@>     GLU335    A        N_3236  <--->     THR332    A      OG1_3192     3.3    39.6
@>     LYS249    A        N_2054  <--->     TYR245    A        O_1999     3.3    26.4
@>     ALA128    A          N_43  <--->     ASP131    A       OD1_97     3.4     4.6
@>     GLU220    A        N_1591  <--->     THR216    A        O_1521     3.4    37.4
@>     VAL309    A        N_2823  <--->     ASP306    A        O_2779     3.4    19.5
@>     TYR218    A        N_1546  <--->     PRO258    A        O_2233     3.4    28.7
@>     GLY197    A        N_1211  <--->     ILE208    A        O_1397     3.4    20.4
@>     ARG254    A        N_2152  <--->     ASP310    A      OD1_2849     3.4    20.2
@>     ASP310    A        N_2839  <--->     GLU307    A        O_2791     3.4    27.3
@>     ALA171    A         N_762  <--->     GLN167    A         O_694     3.4    23.6
@>     VAL181    A         N_926  <--->     ARG178    A         O_868     3.4    34.7
@>     GLY215    A        N_1509  <--->     ALA212    A        O_1471     3.4     6.4
@>     TRP312    A        N_2870  <--->     LYS308    A        O_2806     3.5    22.5
@>     GLN184    A       NE2_990  <--->     ASP273    A      OD1_2459     3.5    17.3
@>     VAL376    A        N_3934  <--->     MET372    A        O_3864     3.5    26.9
@> Number of detected hydrogen bonds: 64.
@> Creating file with dummy atoms
..
..
```

Now, we need to go to the newly created folder `struc_homologs_BLAST` and use `findClusterCenters()` for each type of interactions to detect clusters of interactions. We cannot do it in an automatic way because each system is different and often default parameters of `numC` and `distC` should be tuned.

To compute fingerprint interactions of hydrogen bonds, use the command below. This function uses the prefix `INT_HBs_` to select analyzed interactions. Originally, `findClusterCenters()` was created to analyze water clusters with the WatFinder module. To apply it here, we are changing the `selection` to `resnume DUM` given to dummy atoms that represent interactions.

```
In [4]: findClusterCenters('INT_HBs_*.pdb', selection = 'resname DUM')
```

```
@> 4362 atoms and 1 coordinate set(s) were parsed in 0.11s.
@> 4433 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4122 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4383 atoms and 1 coordinate set(s) were parsed in 0.05s.
```

```
@> 4568 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4594 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4269 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4249 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4205 atoms and 1 coordinate set(s) were parsed in 0.05s.
..
..
@> 4177 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4428 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4245 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4269 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4417 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4610 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> Results are saved in clusters_INT_HBs_.pdb.
```

To compute the fingerprint interactions of salt bridges, use the prefix `INT_SBs_`:

```
In [5]: findClusterCenters('INT_SBs_*.pdb', selection = 'resname DUM')
```

```
@> 4306 atoms and 1 coordinate set(s) were parsed in 0.11s.
@> 4383 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4082 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4337 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4532 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4558 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4228 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4213 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4154 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4303 atoms and 1 coordinate set(s) were parsed in 0.06s.
@> 4350 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4107 atoms and 1 coordinate set(s) were parsed in 0.05s.
..
..
@> 4199 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4233 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4369 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4569 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> Results are saved in clusters_INT_SBs_.pdb.
```

To compute the fingerprint interactions of repulsive ionic bonding, use the prefix `INT_RIB_`:

```
In [6]: findClusterCenters('INT_RIB_*.pdb', selection = 'resname DUM')
```

```
@> 4367 atoms and 1 coordinate set(s) were parsed in 0.11s.
@> 4322 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4510 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4537 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4218 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4199 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4142 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4286 atoms and 1 coordinate set(s) were parsed in 0.05s.
..
..
@> 4353 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4182 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4215 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4351 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4548 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Results are saved in clusters_INT_RIB_.pdb.
```

To compute the fingerprint of pi-stacking interactions, use the prefix `INT_PiStack_`:

```
In [7]: findClusterCenters('INT_PiStack_*.pdb', selection = 'resname DUM')
```

```
@> 4292 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4368 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4066 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4322 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4510 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4536 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4220 atoms and 1 coordinate set(s) were parsed in 0.04s.
..
..
@> 4119 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4354 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4182 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4352 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4548 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Results are saved in clusters_INT_PiStack_.pdb.
```

To compute the fingerprint of pi-stacking interactions, use the prefix `INT_PiCat_`:

```
In [8]: findClusterCenters('INT_PiCat_*.pdb', selection = 'resname DUM')
```

```
@> 4295 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4369 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4068 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4323 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4516 atoms and 1 coordinate set(s) were parsed in 0.05s.
..
..
@> 4184 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4219 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4356 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4551 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> Results are saved in clusters_INT_PiCat_.pdb.
```

To compute the fingerprint of hydrophobic interactions, use the prefix `INT_HPh_`:

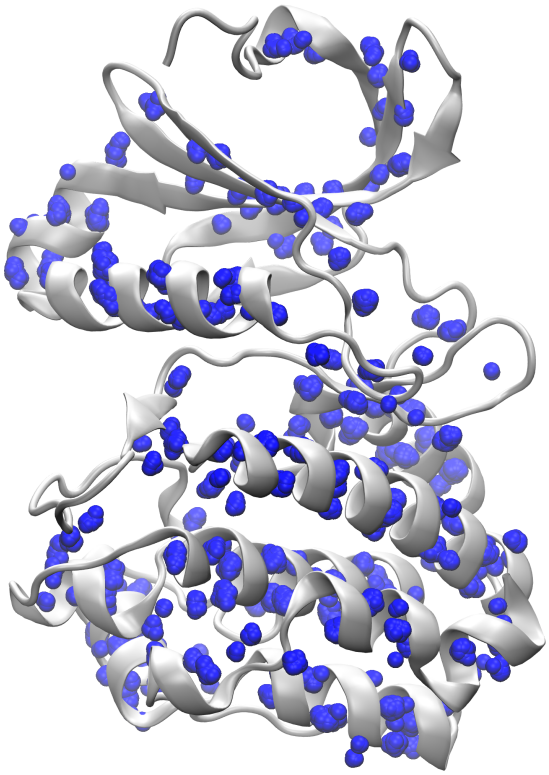
```
In [9]: findClusterCenters('INT_HPh_*.pdb', selection = 'resname DUM')
```

```
@> 4374 atoms and 1 coordinate set(s) were parsed in 0.12s.
@> 4446 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4142 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4398 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4594 atoms and 1 coordinate set(s) were parsed in 0.05s.
..
..
@> 4427 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4260 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4295 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4426 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4625 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Results are saved in clusters_INT_HPh_.pdb.
```

We can further visualize those results in a graphical program like **VMD_**. The obtained results are with default `numC` and `distC` parameters, and it means that we were identifying interactions that were within 0.3 Ang. from each other (`distC`) in at least three structures (`numC`). To see more information about those parameters, see the WatFinder

tutorial[15].

The visualization of hydrogen bond clusters is as follows:



The visualization of salt bridge clusters:

The visualization of repulsive ionic bonding clusters:

The visualization of pi-cation clusters:

The visualization of pi-stacking clusters:

The visualization of hydrophobic clusters:

8.2 Dali approach

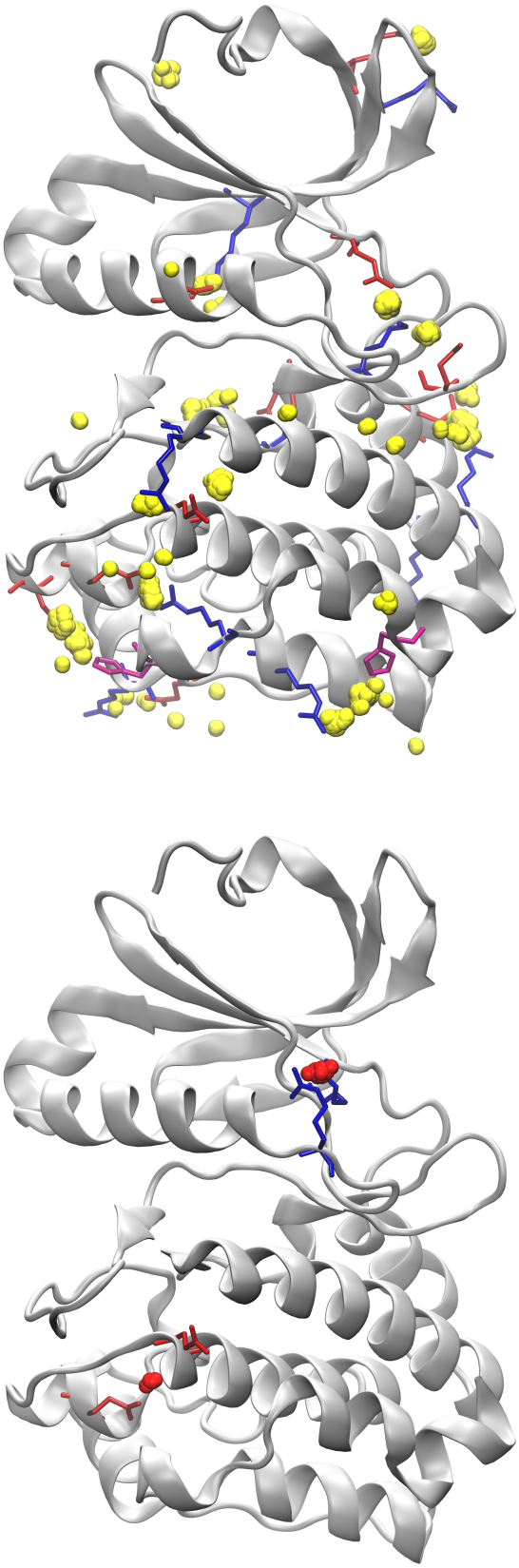
We can use a similar approach with the PDB list provided by the Dali server instead of BLAST. This time, to download homologs, add missing hydrogens, and align structures, we will use `runDali()` function.

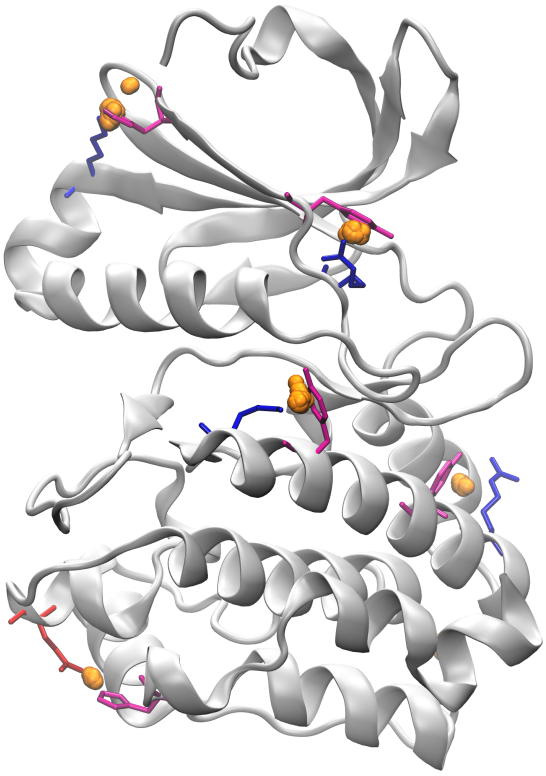
For the `subset_Dali` parameter, we will use `PDB25` instead of the full list of homologs, which is the default.

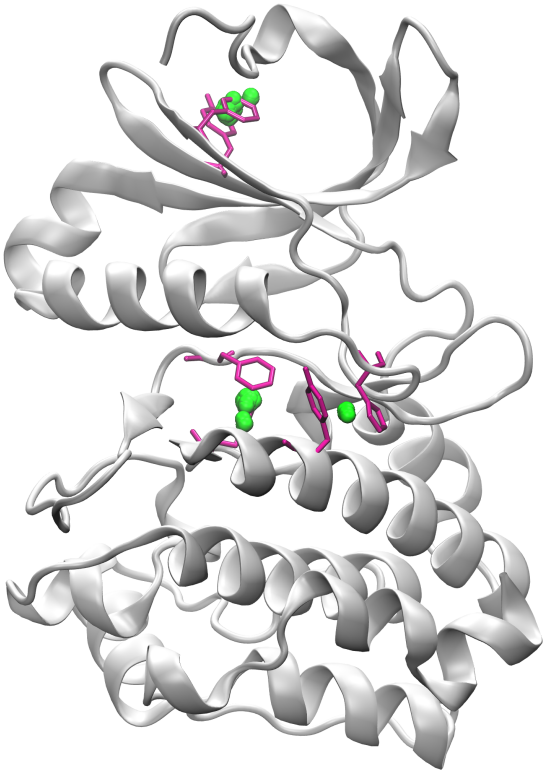
We will use Openbabel to fix the structure and all prepared structures will be copied to a folder with `folder_name` set to `struc_homologs_Dali`.

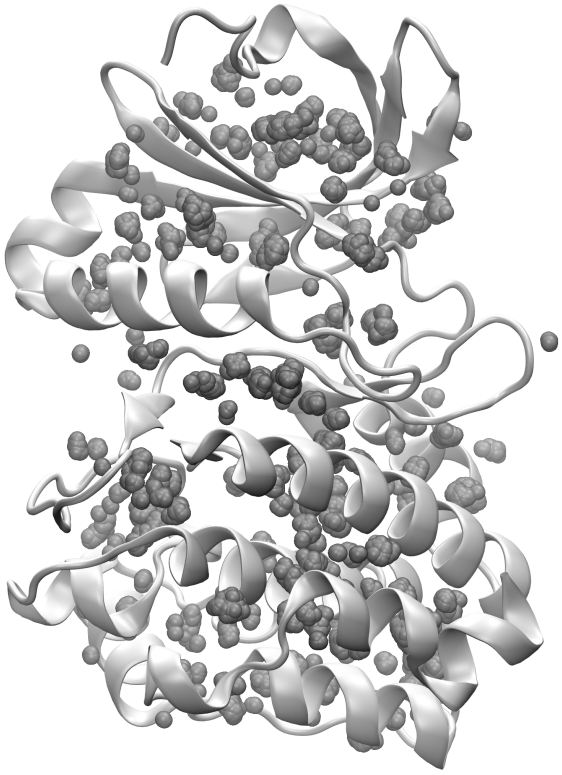
```
In [10]: runDali(PDBcode, 'A', fixer='openbabel', subset_Dali='PDB25',
   ....:         folder_name='struc_homologs_Dali')
   ....:
```

[15] http://www.bahargroup.org/prody/tutorials/watfinder_tutorial









```
@> Submitted Dali search for PDB "1ol5A".
@> http://ekhidna2.biocenter.helsinki.fi/barcosel/tmp//1ol5A/
@> Dali results were fetched in 0.2s.
@> Obtained 158 PDB chains from Dali for 1ol5A.
@> 28 PDBs have been filtered out from 158 Dali hits (remaining: 130).
@> Separating chains and saving into PDB file
@> PDB code 4ysm and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 4ysm downloaded (4ysm.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 7528 atoms and 1 coordinate set(s) were parsed in 0.20s.
@> PDB code 5dzc and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 5dzc downloaded (5dzc.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 6578 atoms and 1 coordinate set(s) were parsed in 0.18s.
@> PDB code 8jpb and chain G
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 8jpb downloaded (8jpb.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 9650 atoms and 1 coordinate set(s) were parsed in 0.14s.
@> PDB code 5u6y and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 5u6y downloaded (5u6y.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
```

```
@> 86921 atoms and 1 coordinate set(s) were parsed in 0.94s.
@> PDB code 7myj and chain C
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 7myj downloaded (7myj.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 14740 atoms and 1 coordinate set(s) were parsed in 0.25s.
@> PDB code 6c9j and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 6c9j downloaded (6c9j.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 7034 atoms and 1 coordinate set(s) were parsed in 0.19s.
@> PDB code 3pfq and chain A
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 3pfq downloaded (3pfq.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 4273 atoms and 1 coordinate set(s) were parsed in 0.12s.
@> PDB code 8qgy and chain B
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 8qgy downloaded (8qgy.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 25443 atoms and 1 coordinate set(s) were parsed in 0.33s.
@> PDB code 5xzw and chain B
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 5xzw downloaded (5xzw.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 5648 atoms and 1 coordinate set(s) were parsed in 0.18s.
@> PDB code 2pml and chain X
..
..
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 9b9g downloaded (9b9g.pdb.gz)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
@> 48664 atoms and 1 coordinate set(s) were parsed in 0.55s.
@> Adding hydrogens to the structures..
@> Hydrogens were added to the structure. New structure is saved as addH_4ysmA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_5dzcA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_8jpbG.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_5u6yA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_7myjC.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_6c9jA.pdb.
..
..
@> Hydrogens were added to the structure. New structure is saved as addH_8fnyA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_4axdA.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_7k10A.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_6z2wE.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_9b9gA.pdb.
@> 130 PDBs were parsed in 11.15s.
@> Aligning the structures..
@> addH_5dzcA
@> Checking AtomGroup addH_5dzcA: 1 chains are identified
@> Checking AtomGroup addH_4ysmA: 1 chains are identified
```

```
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_5dzcA (len=816) and Chain A from addH_4ysmA (len=475):
@>   Match: 468 residues match with 6% sequence identity and 57% overlap.
@> Aligning the structures..
@> addH_8jpbG
@> Checking AtomGroup addH_8jpbG: 1 chains are identified
@> Checking AtomGroup addH_4ysmA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain G from addH_8jpbG (len=658) and Chain A from addH_4ysmA (len=475):
@>   Match: 475 residues match with 8% sequence identity and 72% overlap.
@> Aligning the structures..
@> addH_5u6yA
@> Checking AtomGroup addH_5u6yA: 1 chains are identified
@> Checking AtomGroup addH_4ysmA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_5u6yA (len=459) and Chain A from addH_4ysmA (len=475):
@>   Match: 458 residues match with 8% sequence identity and 96% overlap.
@> Aligning the structures..
@> addH_7myjC
@> Checking AtomGroup addH_7myjC: 1 chains are identified
@> Checking AtomGroup addH_4ysmA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain C from addH_7myjC (len=465) and Chain A from addH_4ysmA (len=475):
@>   Match: 443 residues match with 5% sequence identity and 93% overlap.
@> Aligning the structures..
@> addH_6c9jA
@> Checking AtomGroup addH_6c9jA: 1 chains are identified
@> Checking AtomGroup addH_4ysmA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_6c9jA (len=386) and Chain A from addH_4ysmA (len=475):
@>   Failed to match chains (seqid=5%, overlap=76%).
@> Trying to match chains based on local sequence alignment:
@>  Comparing Chain A from addH_6c9jA (len=386) and Chain A from addH_4ysmA (len=475):
/home/karolamik/.local/lib/python3.10/site-packages/Bio/pairwise2.py:278: BiopythonDeprecationWarning
warnings.warn(
@>   Match: 381 residues match with 35% sequence identity and 80% overlap.
@> Aligning the structures..
@> addH_3pfqA
@> Checking AtomGroup addH_3pfqA: 1 chains are identified
@> Checking AtomGroup addH_4ysmA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_3pfqA (len=523) and Chain A from addH_4ysmA (len=475):
@>   Failed to match chains (seqid=4%, overlap=64%).
@> Trying to match chains based on local sequence alignment:
@>  Comparing Chain A from addH_3pfqA (len=523) and Chain A from addH_4ysmA (len=475):
@>   Match: 334 residues match with 24% sequence identity and 64% overlap.
@> Aligning the structures..
@> addH_8qgyB
@> Checking AtomGroup addH_8qgyB: 1 chains are identified
@> Checking AtomGroup addH_4ysmA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain B from addH_8qgyB (len=809) and Chain A from addH_4ysmA (len=475):
@>   Failed to match chains (seqid=4%, overlap=45%).
@> Trying to match chains based on local sequence alignment:
@>  Comparing Chain B from addH_8qgyB (len=809) and Chain A from addH_4ysmA (len=475):
@>   Match: 457 residues match with 35% sequence identity and 56% overlap.
@> Aligning the structures..
@> addH_5xzwB
```

```
@> Checking AtomGroup addH_5xzwB: 1 chains are identified
@> Checking AtomGroup addH_4ysmA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain B from addH_5xzwB (len=379) and Chain A from addH_4ysmA (len=475):
@>   Match: 379 residues match with 6% sequence identity and 80% overlap.
@> Aligning the structures..
@> addH_2pmlX
@> Checking AtomGroup addH_2pmlX: 1 chains are identified
@> Checking AtomGroup addH_4ysmA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain X from addH_2pmlX (len=340) and Chain A from addH_4ysmA (len=475):
@>   Match: 329 residues match with 10% sequence identity and 69% overlap.
..
..
@> Aligning the structures..
@> addH_7k10A
@> Checking AtomGroup addH_7k10A: 1 chains are identified
@> Checking AtomGroup addH_4ysmA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_7k10A (len=1259) and Chain A from addH_4ysmA (len=475):
@>   Failed to match chains (seqid=0%, overlap=0%).
@> Trying to match chains based on local sequence alignment:
@>  Comparing Chain A from addH_7k10A (len=1259) and Chain A from addH_4ysmA (len=475):
@>   Failed to match chains (seqid=32%, overlap=36%).
@> WARNING There is a problem with addH_7k10A. Change seqid or overlap parameter to include the struc
@> Aligning the structures..
@> addH_6z2wE
@> Checking AtomGroup addH_6z2wE: 1 chains are identified
@> Checking AtomGroup addH_4ysmA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain E from addH_6z2wE (len=2325) and Chain A from addH_4ysmA (len=475):
@>   Failed to match chains (seqid=6%, overlap=20%).
@> Trying to match chains based on local sequence alignment:
@>  Comparing Chain E from addH_6z2wE (len=2325) and Chain A from addH_4ysmA (len=475):
@>   Failed to match chains (seqid=36%, overlap=20%).
@> WARNING There is a problem with addH_6z2wE. Change seqid or overlap parameter to include the struc
@> Aligning the structures..
@> addH_9b9gA
@> Checking AtomGroup addH_9b9gA: 1 chains are identified
@> Checking AtomGroup addH_4ysmA: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_9b9gA (len=1696) and Chain A from addH_4ysmA (len=475):
@>   Failed to match chains (seqid=5%, overlap=19%).
@> Trying to match chains based on local sequence alignment:
@>  Comparing Chain A from addH_9b9gA (len=1696) and Chain A from addH_4ysmA (len=475):
@>   Failed to match chains (seqid=32%, overlap=27%).
@> WARNING There is a problem with addH_9b9gA. Change seqid or overlap parameter to include the struc
```

Further, we can analyze `struc_homologs_Dali` folder with prepared PDB files in a similar way as for the BLAST dataset by using `calcSignatureInteractions()` and `findClusterCenters()` for each interaction type (see the BLAST approach).

```
In [11]: calcSignatureInteractions('struc_homologs_Dali')
```

```
@> struc_homologs_Dali/align__addH_6yb8A.pdb
@> 6563 atoms and 1 coordinate set(s) were parsed in 0.07s.
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
```

@>	ASN184	A	N_2817	<--->	LEU181	A	O_2772	2.8	7.3
@>	ILE411	A	N_6306	<--->	LEU407	A	O_6240	2.8	32.4
@>	ALA387	A	N_5916	<--->	SER383	A	O_5863	2.8	34.0
@>	ALA88	A	N_1278	<--->	VAL31	A	O_401	2.9	34.0
@>	PHE121	A	N_1812	<--->	ARG102	A	O_1509	2.9	29.2
@>	SER349	A	N_5373	<--->	SER375	A	O_5756	2.9	33.9
@>	SER383	A	OG_5867	<--->	PRO380	A	O_5826	2.9	28.3
@>	LYS178	A	N_2710	<--->	GLU174	A	O_2647	2.9	36.2
@>	VAL196	A	N_3003	<--->	GLU92	A	O_1335	2.9	38.7
@>	CYS350	A	N_5384	<--->	ALA327	A	O_5080	2.9	36.4
@>	ASN43	A	ND2_590	<--->	ASN136	A	OD1_2073	2.9	5.6
@>	GLU174	A	N_2642	<--->	GLN170	A	O_2581	2.9	34.3
@>	GLY305	A	N_4743	<--->	SER301	A	O_4688	2.9	33.3
@>	ASP163	A	N_2476	<--->	GLN159	A	O_2419	2.9	17.6
@>	VAL162	A	N_2460	<--->	GLY158	A	O_2413	2.9	31.4
@>	SER166	A	N_2524	<--->	VAL162	A	O_2465	2.9	37.4
@>	VAL204	A	N_3131	<--->	GLY195	A	O_3002	2.9	29.1
@>	LYS59	A	N_817	<--->	ALA55	A	O_768	2.9	22.4
@>	ASN136	A	N_2063	<--->	ASP133	A	O_2032	2.9	17.8
@>	ILE94	A	N_1362	<--->	PHE194	A	O_2981	2.9	38.6
@>	LYS418	A	N_6416	<--->	LYS414	A	O_6360	2.9	5.8
@>	THR61	A	N_858	<--->	SER57	A	O_797	3.0	22.5
@>	GLY341	A	N_5258	<--->	PRO337	A	O_5204	3.0	35.1
@>	ILE192	A	N_2942	<--->	TRP98	A	O_1434	3.0	28.5
@>	GLU250	A	N_3886	<--->	LYS246	A	O_3813	3.0	29.9
@>	ALA253	A	N_3941	<--->	PHE249	A	O_3871	3.0	30.3
@>	GLU317	A	N_4935	<--->	LYS313	A	O_4872	3.0	16.3
@>	GLN144	A	N_2185	<--->	SER141	A	OG_2153	3.0	12.3
@>	LYS125	A	N_1881	<--->	ARG101	A	O_1485	3.0	38.6
@>	LYS246	A	N_3808	<--->	LEU242	A	O_3744	3.0	33.3
@>	THR409	A	N_6268	<--->	SER405	A	O_6210	3.0	1.5
@>	HIS167	A	N_2535	<--->	ASP163	A	O_2481	3.0	33.2
@>	ARG46	A	NH1_631	<--->	TYR231	A	O_3565	3.0	23.7
@>	ALA314	A	N_4889	<--->	LEU310	A	O_4810	3.0	36.2
@>	SER349	A	OG_5382	<--->	ASN333	A	ND2_5164	3.0	24.2
@>	VAL324	A	N_5023	<--->	ARG267	A	O_4170	3.0	34.6
@>	LYS419	A	N_6438	<--->	GLN415	A	O_6382	3.0	23.6
@>	ARG111	A	N_1650	<--->	SER107	A	O_1583	3.0	29.5
@>	ASN248	A	N_3852	<--->	MET244	A	O_3780	3.0	31.1
@>	ILE406	A	N_6216	<--->	LEU402	A	O_6157	3.0	23.2
@>	GLY72	A	N_1030	<--->	GLN69	A	O_993	3.0	28.6
@>	ALA147	A	N_2240	<--->	GLU143	A	O_2175	3.0	20.6
@>	GLY241	A	N_3732	<--->	THR238	A	OG1_3697	3.0	23.3
@>	GLN224	A	N_3442	<--->	ASP221	A	O_3400	3.0	19.9
@>	VAL188	A	N_2875	<--->	ARG215	A	O_3301	3.0	23.0
@>	THR309	A	N_4791	<--->	GLY305	A	O_4749	3.0	31.8
@>	PHE173	A	N_2622	<--->	THR169	A	O_2567	3.0	1.9
@>	ARG421	A	NH1_6497	<--->	ASP417	A	OD2_6415	3.0	38.6
@>	LEU402	A	N_6152	<--->	VAL398	A	O_6084	3.0	18.5
@>	ILE390	A	N_5953	<--->	PHE386	A	O_5901	3.0	15.4
@>	TRP399	A	N_6095	<--->	ASN395	A	O_6034	3.0	31.4
@>	SER394	A	N_6018	<--->	PHE391	A	O_5977	3.0	36.8
@>	LYS414	A	N_6355	<--->	TRP410	A	O_6287	3.0	17.7
@>	ALA206	A	N_3166	<--->	GLU193	A	O_2966	3.0	13.9
@>	VAL268	A	N_4189	<--->	PRO294	A	O_4574	3.1	28.0
@>	VAL21	A	N_240	<--->	TYR14	A	O_129	3.1	25.1
@>	ARG111	A	NH1_1668	<--->	SER107	A	OG_1587	3.1	32.8
@>	ILE56	A	N_773	<--->	GLY52	A	O_730	3.1	15.0

```
@>     ARG311    A        N_4824  <--->     ASP307    A        O_4769     3.1    33.3
@>     LEU259    A        N_4040  <--->     VAL256    A        O_3995     3.1    29.7
@>     VAL198    A        N_3031  <--->      GLN90    A        O_1307     3.1    31.9
@>     LEU242    A        N_3739  <--->     THR238    A        O_3694     3.1     5.5
@>     LYS285    A        N_4438  <--->     CYS281    A        O_4376     3.1    32.4
@>     MET165    A        N_2507  <--->     GLU161    A        O_2450     3.1    24.8
@>      LEU32    A         N_412  <--->      TYR22    A         O_261     3.1    31.8
@>     LYS228    A        N_3510  <--->     ASN211    A        O_3240     3.1    27.9
@>     ASP197    A        N_3019  <--->     GLU202    A        O_3102     3.1    13.8
@>     PHE391    A        N_5972  <--->     ALA387    A        O_5921     3.1    19.4
@>     ASP277    A        N_4316  <--->     SER274    A        O_4285     3.1    21.7
@>     PHE325    A        N_5039  <--->     PRO346    A        O_5328     3.1    35.1
@>     VAL377    A        N_5776  <--->     SER349    A        O_5378     3.1    35.0
@>     GLY289    A        N_4503  <--->     LYS285    A        O_4443     3.1    37.5
@>     GLU315    A        N_4899  <--->     ARG311    A        O_4829     3.1    27.0
@>       ASN8    A          N_21  <--->      ASP26    A      OD2_341      3.1    25.4
@>     ALA148    A        N_2250  <--->     GLN144    A        O_2190     3.1    16.0
@>     LYS304    A        N_4721  <--->     SER301    A       OG_4692     3.1    19.1
@>      GLY10    A          N_54  <--->      GLU23    A         O_282     3.1    33.5
@>     ALA171    A        N_2593  <--->     HIS167    A        O_2540     3.1    11.4
@>     LEU216    A        N_3320  <--->     ASP227    A      OD1_3508     3.1    27.7
@>     TRP410    A        N_6282  <--->     ILE406    A        O_6221     3.1    26.6
@>      GLU23    A         N_277  <--->      LYS11    A          O_66     3.1    20.8
@>     LYS401    A        N_6130  <--->     LEU397    A        O_6065     3.2    17.9
@>     CYS281    A        N_4371  <--->     ASP277    A        O_4321     3.2    15.2
@>     LYS226    A        N_3476  <--->     LEU216    A        O_3325     3.2    39.6
@>     LEU310    A        N_4805  <--->     PRO306    A        O_4754     3.2    10.6
@>      ALA71    A        N_1020  <--->      LEU67    A         O_955     3.2    11.3
@>      PHE86    A        N_1239  <--->      LEU33    A         O_436     3.2    34.3
@>      LEU25    A         N_311  <--->       ASN8    A          O_26     3.2    29.8
@>      SER27    A         N_342  <--->      LEU24    A         O_297     3.2    21.1
@>     LEU413    A        N_6336  <--->     THR409    A        O_6273     3.2    11.0
@>     VAL245    A        N_3792  <--->     GLY241    A        O_3738     3.2    16.2
@>     ARG215    A        N_3296  <--->     ASP189    A        O_2896     3.2    34.7
@>     GLY118    A        N_1762  <--->     ALA104    A        O_1552     3.2    36.9
@>     LYS149    A        N_2260  <--->     ILE146    A        O_2226     3.2    11.1
@>     LEU407    A        N_6235  <--->     ARG403    A        O_6176     3.2    17.0
@>      LYS17    A        NZ_185  <--->     ASP133    A      OD2_2038     3.2    27.2
@>     ASN112    A        N_1674  <--->     LEU109    A        O_1614     3.3    35.6
@>     ASN290    A        N_4510  <--->     LYS286    A        O_4465     3.3    32.4
@>     GLN159    A      NE2_2428  <--->     ASP163    A      OD2_2487     3.3    34.8
@>     TYR119    A        N_1769  <--->     LYS116    A        O_1730     3.3     9.8
@>     GLY392    A        N_5992  <--->     GLN389    A        O_5941     3.3    32.8
@>     GLN243    A        N_3758  <--->     PRO239    A        O_3707     3.3    17.0
@>     LEU145    A        N_2202  <--->     SER141    A        O_2149     3.3     9.6
@>     HIS280    A      NE2_4369  <--->     CYS350    A       SG_5393     3.3    39.9
@>     LEU234    A        N_3617  <--->     TYR231    A        O_3565     3.3    28.0
@>     ILE103    A        N_1528  <--->     VAL188    A        O_2880     3.3    37.2
@>     MET244    A        N_3775  <--->     GLU240    A        O_3722     3.3    28.9
@>      ASN58    A       ND2_814  <--->      GLY82    A        O_1199     3.4    35.5
@>     THR200    A      OG1_3069  <--->     ASP197    A      OD1_3029     3.4     4.3
@>      ARG46    A       NH2_634  <--->     LYS235    A        O_3641     3.4    27.6
@>     ASN342    A        N_5265  <--->     VAL338    A        O_5219     3.4    34.2
@>     LEU181    A        N_2767  <--->     GLU177    A        O_2700     3.4     7.3
@>     GLN170    A        N_2576  <--->     SER166    A        O_2529     3.4    12.9
@>     TYR316    A        N_4914  <--->     ILE312    A        O_4853     3.4    24.9
@>     GLU202    A        N_3097  <--->     THR200    A      OG1_3069     3.4    34.6
@>     ASN424    A        N_6529  <--->     ARG421    A        O_6484     3.4    23.2
```

```
@>      LEU68    A         N_969  <--->      PHE65    A         O_918     3.4    37.0
@>      ARG79    A        N_1136  <--->      ILE87    A        O_1264     3.4    25.5
@>     ALA384    A        N_5869  <--->     PRO380    A        O_5826     3.4    36.1
@>      LYS53    A         N_731  <--->      LEU50    A         O_695     3.4    39.7
@>     HIS396    A        N_6043  <--->     GLU263    A      OE1_4124     3.4    14.8
@>     ILE284    A        N_4419  <--->     HIS280    A        O_4359     3.5    29.6
@> Number of detected hydrogen bonds: 122.
@> Creating file with dummy atoms
@> struc_homologs_Dali/align__addH_8uw7A.pdb
@> 6534 atoms and 1 coordinate set(s) were parsed in 0.08s.
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      VAL57    A         N_820  <--->      GLY33    A         O_542     2.8    35.2
@>     LEU202    A        N_2866  <--->     ASN199    A        O_2817     2.8    30.9
@>     PHE245    A        N_3579  <--->     MET342    A        O_4924     2.8    31.3
@>     LYS420    A        N_6207  <--->     HIS415    A        O_6121     2.8    37.6
@>     MET118    A        N_1817  <--->     GLU114    A        O_1762     2.8    28.8
@>     ARG222    A      NH1_3216  <--->     ASP221    A        O_3191     2.9    34.5
@>     ILE290    A        N_4318  <--->     PHE209    A        O_2987     2.9    29.4
@>     GLN218    A      NE2_3152  <--->     GLU198    A      OE2_2811     2.9    35.2
@>     MET281    A        N_4171  <--->     LYS289    A        O_4301     2.9    10.3
@>     MET339    A        N_4866  <--->     LEU335    A        O_4813     2.9    40.0
@>     ARG241    A        N_3500  <--->     PHE237    A        O_3438     2.9    31.1
@>     THR100    A        N_1544  <--->      ARG96    A        O_1471     2.9    24.7
@>     ASP108    A        N_1658  <--->     GLN104    A        O_1606     2.9    21.1
@>     ARG391    A       NE_5755  <--->     LYS385    A        O_5636     2.9    34.7
@>     LEU335    A        N_4808  <--->     ASP331    A        O_4746     2.9    39.1
@>     VAL337    A        N_4834  <--->     TRP333    A        O_4782     2.9    27.5
@>     LYS111    A        N_1696  <--->     ALA107    A        O_1653     2.9    37.3
@>     ILE103    A        N_1582  <--->      TRP99    A        O_1525     2.9    39.7
@>     LEU181    A        N_2595  <--->     LEU223    A        O_3227     2.9    37.2
@>     TYR340    A        N_4883  <--->     GLY336    A        O_4833     2.9    38.7
@>     LYS170    A        N_2408  <--->     GLU149    A        O_2057     2.9    31.2
@>     SER381    A        N_5575  <--->     LYS377    A        O_5509     2.9    35.5
@>      GLY33    A         N_536  <--->      LYS30    A         O_493     2.9    31.2
@>     ARG391    A      NH1_5758  <--->     ALA329    A        O_4720     2.9    24.4
@>     THR105    A        N_1618  <--->     THR101    A        O_1563     2.9    34.5
@>     VAL271    A        N_3990  <--->      ASN54    A       OD1_785     2.9    10.3
@>     LEU264    A        N_3876  <--->     ALA260    A        O_3819     2.9    33.9
@>     SER378    A        N_5526  <--->     PRO374    A        O_5469     3.0     9.1
@>      THR65    A         N_949  <--->      THR72    A        O_1073     3.0    24.5
@>     GLN104    A        N_1601  <--->     THR100    A        O_1549     3.0    39.3
@>     SER259    A        N_3803  <--->     ALA255    A        O_3748     3.0    37.2
@>     LEU235    A        N_3394  <--->     LEU280    A        O_4157     3.0    30.2
@>     GLY393    A        N_5783  <--->     GLU401    A      OE1_5887     3.0    11.8
@>     GLU322    A        N_4610  <--->     PRO318    A        O_4550     3.0    36.4
@>     HIS238    A        N_3453  <--->     GLU234    A        O_3384     3.0    32.5
@>     LEU357    A        N_5166  <--->     ASP353    A        O_5105     3.0    30.9
@>      GLU97    A        N_1490  <--->      PRO93    A        O_1426     3.0    33.8
@>     ALA107    A        N_1648  <--->     ILE103    A        O_1587     3.0    20.9
@>     TYR417    A        N_6149  <--->     TRP413    A        O_6080     3.0    27.9
@>      THR82    A        N_1238  <--->      GLN79    A        O_1188     3.1    31.2
@>     TYR215    A        N_3086  <--->     VAL226    A        O_3277     3.1    37.3
@>     GLU228    A        N_3305  <--->     ALA212    A        O_3040     3.1    36.8
@>     GLU418    A        N_6170  <--->     GLN414    A        O_6104     3.1    23.2
@>     GLY373    A        N_5458  <--->     GLU247    A      OE2_3624     3.1    10.3
@>     TYR263    A        N_3855  <--->     SER259    A        O_3808     3.1    15.6
@>     TYR253    A        N_3715  <--->     ARG249    A        O_3642     3.1    33.1
```

```
@>      GLY157    A        N_2202  <--->      VAL164    A        O_2306     3.1    32.3
@>       ARG96    A        N_1466  <--->       THR92    A        O_1413     3.1    29.8
@>      LEU110    A        N_1677  <--->      VAL106    A        O_1637     3.1    30.4
@>      ALA260    A        N_3814  <--->      GLU256    A        O_3758     3.1    15.7
@>      ASP331    A        N_4741  <--->      ARG328    A        O_4696     3.1    38.1
@>      THR100    A      OG1_1552  <--->       GLU97    A        O_1495     3.2    30.9
@>      GLY109    A        N_1670  <--->      THR105    A        O_1623     3.2    32.6
@>       ARG15    A         N_201  <--->       THR87    A        O_1331     3.2    16.5
@>      GLU256    A        N_3753  <--->      PHE252    A        O_3700     3.2     5.4
@>      VAL187    A        N_2708  <--->      LYS183    A        O_2641     3.2    17.5
@>      TRP333    A        N_4777  <--->      ALA329    A        O_4720     3.2    31.9
@>      GLU359    A        N_5205  <--->      GLU355    A        O_5134     3.2     8.1
@>       GLU98    A        N_1505  <--->       GLU94    A        O_1441     3.2    15.5
@>      GLY334    A        N_4801  <--->      VAL330    A        O_4730     3.2    31.0
@>       PHE55    A         N_789  <--->       LEU52    A         O_747     3.3    28.2
@>      PHE150    A        N_2067  <--->      MET147    A        O_2026     3.3    17.7
@>      ILE186    A        N_2689  <--->      LYS183    A        O_2641     3.3    22.2
@>      ARG391    A        N_5740  <--->      PRO388    A        O_5691     3.3    23.0
@>      GLU116    A        N_1787  <--->      LYS112    A        O_1723     3.3    23.9
@>      HIS405    A        N_5942  <--->      GLU401    A        O_5879     3.3    23.5
@>      HIS265    A        N_3895  <--->      ASP262    A        O_3848     3.3    38.1
@>      ARG243    A        N_3539  <--->      SER240    A        O_3494     3.3    13.1
@>      ASN231    A      ND2_3362  <--->      ASP434    A        O_6435     3.4     9.2
@>       ARG86    A      NH2_1323  <--->       PHE55    A         O_794     3.4    32.9
@>       VAL90    A        N_1377  <--->       ASN71    A        O_1059     3.4    19.9
@>      TYR315    A        N_4496  <--->      THR312    A        O_4458     3.4    15.4
@>       THR72    A      OG1_1076  <--->       ARG69    A        O_1021     3.4    36.8
@>      GLU242    A        N_3524  <--->      LEU239    A        O_3475     3.4    31.5
@>      LEU384    A        N_5612  <--->      SER381    A        O_5580     3.4    31.7
@>      VAL185    A        N_2673  <--->      LYS182    A        O_2619     3.5    30.9
@> Number of detected hydrogen bonds: 76.
@> Creating file with dummy atoms
..
..
```

8.3 Foldseek approach

Foldseek requires additional installation of Foldseek and the PDB database download. See more details on the Foldseek[16] website. Once the installation of Foldseek and downloading database to `~/Downloads/foldseek` folder is done, we can run `runFoldseek()` function. Foldseek requires a PDB file in the local directory. Therefore, first, we will fetch it.

```
In [12]: fetchPDB(PDBcode, compressed=False)
```

```
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> Downloading PDB files via FTP failed, trying HTTP.
@> 1ol5 downloaded (1ol5.pdb)
@> PDB download via HTTP completed (1 downloaded, 0 failed).
```

Now, we will run Foldseek, but with more restricted parameters by applying higher values for `coverage_threshold` and `tm_threshold`. Default criteria is providing large number of PDB files for analysis (~4000 files for PDB code 1OL5).

```
In [13]: runFoldseek('1ol5.pdb', 'A', coverage_threshold=0.9, tm_threshold=0.9,
   ....:             database_folder='/home/karolamik/Downloads/foldseek/pdb')
   ....:
```

[16] https://github.com/steineggerlab/foldseek

```
Create directory tmp2
easy-search inp.pdb ~/Downloads/foldseek/pdb prot.foldseek tmp2 --exhaustive-search 1 --format-output

MMseqs Version:                     9.427df8a
Seq. id. threshold                  0
Coverage threshold                  0.9
Coverage mode                       0
Max reject                          2147483647
Max accept                          2147483647
Add backtrace                       false
TMscore threshold                   0
TMalign hit order                   0
TMalign fast                        1
Preload mode                        0
Threads                             12
Verbosity                           3
LDDT threshold                      0
Sort by structure bit score         1
Alignment type                      2
Exact TMscore                       0
Substitution matrix                 aa:3di.out,nucl:3di.out
Alignment mode                      3
Alignment mode                      0
E-value threshold                   10
Min alignment length                0
Seq. id. mode                       0
Alternative alignments              0
Max sequence length                 65535
Compositional bias                  1
Compositional bias                  1
Gap open cost                       aa:10,nucl:10
Gap extension cost                  aa:1,nucl:1
Compressed                          0
Seed substitution matrix            aa:3di.out,nucl:3di.out
Sensitivity                         9.5
k-mer length                        6
Target search mode                  0
k-score                             seq:2147483647,prof:2147483647
Max results per query               1000
Split database                      0
Split mode                          2
Split memory limit                  0
Diagonal scoring                    true
Exact k-mer matching                0
Mask residues                       0
Mask residues probability           0.99995
Mask lower case residues            1
Minimum diagonal score              30
Selected taxa
Spaced k-mers                       1
Spaced k-mer pattern
Local temporary path
Exhaustive search mode              true
Prefilter mode                      0
Search iterations                   1
Remove temporary files              true
MPI runner
```

```
Force restart with latest tmp        false
Cluster search                       0
Path to ProstT5
Chain name mode                      0
Write mapping file                   0
Mask b-factor threshold              0
Coord store mode                     2
Write lookup file                    1
Input format                         0
File Inclusion Regex                 .*
File Exclusion Regex                 ^$
Alignment format                     0
Format alignment output              query,target,qstart,qend,tstart,tend,qcov,tcov,qtmscore,ttmscore
Database output                      false
Greedy best hits                     false

Alignment backtraces will be computed, since they were requested by output format.
createdb inp.pdb tmp2/13199197767129585930/query --chain-name-mode 0 --write-mapping 0 --mask-bfactor

Output file: tmp2/13199197767129585930/query
[=================================================================] 100.00% 1 eta -
Time for merging to query_ss: 0h 0m 0s 0ms
Time for merging to query_h: 0h 0m 0s 0ms
Time for merging to query_ca: 0h 0m 0s 0ms
Time for merging to query: 0h 0m 0s 0ms
Ignore 0 out of 1.
Too short: 0, incorrect: 0, not proteins: 0.
Time for processing: 0h 0m 0s 10ms
Create directory tmp2/13199197767129585930/search_tmp
search tmp2/13199197767129585930/query ~/Downloads/foldseek/pdb tmp2/13199197767129585930/result tmp2

structurealign tmp2/13199197767129585930/query ~/Downloads/foldseek/pdb tmp2/13199197767129585930/sea

[=================================================================] 100.00% 1 eta -
Time for merging to strualn: 0h 0m 0s 0ms
Time for processing: 0h 0m 4s 364ms
mvdb tmp2/13199197767129585930/search_tmp/669226806076435380 9/strualn tmp2/13199197767129585930/searc

Time for processing: 0h 0m 0s 0ms
mvdb tmp2/13199197767129585930/search_tmp/669226806076435380 9/aln tmp2/13199197767129585930/result -v

Time for processing: 0h 0m 0s 0ms
Removing temporary files
rmdb tmp2/13199197767129585930/search_tmp/669226806076435380 9/pref -v 3

Time for processing: 0h 0m 0s 0ms
convertalis tmp2/13199197767129585930/query ~/Downloads/foldseek/pdb tmp2/13199197767129585930/result

[=================================================================] 100.00% 1 eta -
Time for merging to prot.foldseek: 0h 0m 0s 0ms
Time for processing: 0h 0m 6s 547ms
rmdb tmp2/13199197767129585930/result -v 3

Time for processing: 0h 0m 0s 0ms
rmdb tmp2/13199197767129585930/query -v 3

Time for processing: 0h 0m 0s 0ms
rmdb tmp2/13199197767129585930/query_h -v 3
```

```
Time for processing: 0h 0m 0s 0ms
rmdb tmp2/13199197767129585930/query_ca -v 3

Time for processing: 0h 0m 0s 0ms
rmdb tmp2/13199197767129585930/query_ss -v 3

Time for processing: 0h 0m 0s 0ms
@> MSA file is now created, and saved as prot_struc.msa.
--2024-11-29 22:53:23--  https://files.rcsb.org/download/6vpg.pdb
Resolving files.rcsb.org (files.rcsb.org)... 132.249.213.241
Connecting to files.rcsb.org (files.rcsb.org)|132.249.213.241|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: unspecified [application/octet-stream]
Saving to: 'temp/6vpg.pdb'

6vpg.pdb                                [       <=>

2024-11-29 22:53:26 (277 KB/s) - 'temp/6vpg.pdb' saved [430920]

Mismatch in sequence and structure of Target protein 6vpgA at Line 1477 Index 165-None ne T
--2024-11-29 22:53:26--  https://files.rcsb.org/download/7ztl.pdb
Resolving files.rcsb.org (files.rcsb.org)... 132.249.213.241
Connecting to files.rcsb.org (files.rcsb.org)|132.249.213.241|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: unspecified [application/octet-stream]
Saving to: 'temp/7ztl.pdb'

7ztl.pdb                                [        <=>

2024-11-29 22:53:29 (185 KB/s) - 'temp/7ztl.pdb' saved [462186]

Mismatch in sequence and structure of Target protein 7ztlA at Line 1320 Index 162-None ne T
--2024-11-29 22:53:29--  https://files.rcsb.org/download/1mq4.pdb
Resolving files.rcsb.org (files.rcsb.org)... 132.249.213.241
Connecting to files.rcsb.org (files.rcsb.org)|132.249.213.241|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: unspecified [application/octet-stream]
Saving to: 'temp/1mq4.pdb'

1mq4.pdb                                [     <=>

2024-11-29 22:53:31 (217 KB/s) - 'temp/1mq4.pdb' saved [228501]

--2024-11-29 22:53:31--  https://files.rcsb.org/download/5dt3.pdb
Resolving files.rcsb.org (files.rcsb.org)... 132.249.213.241
Connecting to files.rcsb.org (files.rcsb.org)|132.249.213.241|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: unspecified [application/octet-stream]
Saving to: 'temp/5dt3.pdb'

5dt3.pdb                                [     <=>

2024-11-29 22:53:34 (180 KB/s) - 'temp/5dt3.pdb' saved [225666]

Mismatch in sequence and structure of Target protein 5dt3A at Line 1313 Index 160-None ne T
--2024-11-29 22:53:34--  https://files.rcsb.org/download/2w1g.pdb
Resolving files.rcsb.org (files.rcsb.org)... 132.249.213.241
Connecting to files.rcsb.org (files.rcsb.org)|132.249.213.241|:443... connected.
```

```
HTTP request sent, awaiting response... 200 OK
Length: unspecified [application/octet-stream]
Saving to: 'temp/2w1g.pdb'

2w1g.pdb                                [            <=>

2024-11-29 22:53:41 (33,3 KB/s) - 'temp/2w1g.pdb' saved [220077]

--2024-11-29 22:53:41--  https://files.rcsb.org/download/5dpv.pdb
Resolving files.rcsb.org (files.rcsb.org)... 132.249.213.241
Connecting to files.rcsb.org (files.rcsb.org)|132.249.213.241|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: unspecified [application/octet-stream]
Saving to: 'temp/5dpv.pdb'
..
..
@> Individual models are saved in struc_homologs.
@> Adding hydrogens to the structures..
@> Hydrogens were added to the structure. New structure is saved as addH_model1.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_model2.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_model3.pdb.
@> Hydrogens were added to the structure. New structure is saved as addH_model4.pdb.
..
..
@> 87 PDBs were parsed in 3.40s.
@> Aligning the structures..
@> addH_model2
@> Checking AtomGroup addH_model2: 1 chains are identified
@> Checking AtomGroup addH_model1: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_model2 (len=260) and Chain A from addH_model1 (len=264):
@>   Match: 259 residues match with 100% sequence identity and 98% overlap.
@> Aligning the structures..
@> addH_model3
@> Checking AtomGroup addH_model3: 1 chains are identified
@> Checking AtomGroup addH_model1: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_model3 (len=252) and Chain A from addH_model1 (len=264):
@>   Match: 252 residues match with 100% sequence identity and 95% overlap.
@> Aligning the structures..
@> addH_model4
@> Checking AtomGroup addH_model4: 1 chains are identified
@> Checking AtomGroup addH_model1: 1 chains are identified
@> Trying to match chains based on residue numbers and names:
@>   Comparing Chain A from addH_model4 (len=255) and Chain A from addH_model1 (len=264):
@>   Match: 255 residues match with 100% sequence identity and 97% overlap.
@> Aligning the structures..
..
..
```

Once the folder with PDB files will be created, we can analyze it with `calcSignatureInteractions()` and `findClusterCenters()`. Foldseek along with the folder containing PDB files, also generates an MSA file that can be used to obtain sequentially conserved pairs of residues that are corresponding to the interacation types. Therefore, we can analyze only the folder or the folder with the MSA file by giving `mapping_file`. Both cases are shown below. Using the MSA allows us to compare interactions between corresponding residues rather than just comparing in 3D space as above.

Analysis of the folder with prepared PDB homologs:

```
In [14]: calcSignatureInteractions('struc_homologs')
```

```
@> struc_homologs/align__addH_model65.pdb
@> 4126 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)    <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     ARG357    A       NE_3612  <--->     VAL352    A         O_3540     2.7    38.9
@>     LEU225    A        N_1656  <--->     GLU221    A         O_1588     2.8    32.6
@>     ALA150    A         N_372  <--->     LEU159    A          O_537     2.8    30.0
@>     ARG357    A        N_3597  <--->     THR353    A         O_3556     2.9    30.8
@>     LEU159    A         N_532  <--->     ALA150    A          O_377     2.9    29.3
@>     LEU149    A         N_353  <--->     ARG137    A          O_165     2.9    15.6
@>     ARG371    A       NE_3854  <--->     LYS365    A         O_3749     2.9    37.3
@>     MET373    A        N_3877  <--->     GLU376    A       OE1_3950     2.9     2.4
@>     TYR338    A        N_3283  <--->     TYR334    A         O_3221     2.9    20.2
@>     GLU239    A        N_1888  <--->     THR235    A         O_1825     2.9    31.3
@>     CYS319    A        N_2984  <--->     LEU315    A         O_2928     2.9    20.3
@>     VAL344    A        N_3404  <--->     ILE341    A         O_3355     2.9    39.6
@>     VAL163    A         N_602  <--->     ASN146    A          O_307     3.0    29.5
@>     ALA160    A         N_551  <--->     CYS210    A         O_1416     3.0    22.2
@>     LEU169    A         N_706  <--->     PHE165    A          O_642     3.0    36.1
@>     GLU321    A        N_3016  <--->     VAL317    A         O_2954     3.0    30.5
@>     LYS224    A        N_1634  <--->     ARG220    A         O_1564     3.0    23.9
@>     HIS380    A        N_4002  <--->     VAL377    A         O_3957     3.0    19.8
@>     VAL317    A        N_2949  <--->     TRP313    A         O_2893     3.0    27.3
@>     TYR246    A        N_1986  <--->     ASN242    A         O_1937     3.0    34.8
@>     ASN242    A        N_1932  <--->     THR238    A         O_1879     3.0    27.4
@>     ILE209    A        N_1392  <--->     GLY198    A         O_1217     3.1    27.2
@>     THR238    A        N_1874  <--->     ALA234    A         O_1815     3.1    32.0
@>     CYS247    A        N_2007  <--->     ALA243    A         O_1951     3.1    36.4
@>     TYR246    A       OH_2005  <--->     ARG189    A         N_1040     3.1    28.4
@>     ALA243    A        N_1946  <--->     GLU239    A         O_1893     3.1    15.4
@>     ALA385    A        N_4090  <--->     PRO381    A         O_4023     3.1    26.6
@>     TYR148    A         N_332  <--->     LEU161    A          O_566     3.1    34.4
@>     SER361    A        N_3671  <--->     ARG357    A         O_3602     3.1    14.6
@>     LEU296    A        N_2614  <--->     LEU293    A         O_2567     3.1    25.1
@>     ILE360    A        N_3652  <--->     ALA356    A         O_3592     3.1    31.3
@>     LEU315    A        N_2923  <--->     ASP311    A         O_2862     3.1    26.1
@>     GLN223    A        N_1617  <--->     TYR219    A         O_1543     3.1    18.3
@>     LYS250    A        N_2046  <--->     TYR246    A         O_1991     3.1    38.7
@>     GLU336    A        N_3254  <--->     THR333    A       OG1_3210     3.1    27.3
@>     THR235    A        N_1820  <--->     GLN231    A         O_1760     3.1    31.5
@>     SER249    A        N_2035  <--->     SER245    A         O_1980     3.2    13.1
@>     SER314    A        N_2912  <--->     VAL310    A         O_2846     3.2    20.2
@>     LYS250    A       NZ_2064  <--->     HIS187    A         O_1009     3.2    22.6
@>     ASP202    A        N_1276  <--->     ARG205    A         O_1317     3.2    32.9
@>     TYR320    A        N_2995  <--->     GLY316    A         O_2948     3.2    26.2
@>     TYR219    A        N_1538  <--->     PRO259    A         O_2225     3.2    18.1
@>     LEU359    A        N_3633  <--->     GLY355    A         O_3586     3.2     5.7
@>     LEU363    A        N_3706  <--->     LEU359    A         O_3638     3.2    29.4
@>     ALA129    A          N_43  <--->     ASP132    A         OD2_98     3.3    33.5
@>     VAL352    A        N_3535  <--->     PRO349    A         O_3493     3.3    28.8
@>     GLY316    A        N_2942  <--->     LEU312    A         O_2874     3.3    31.9
@>     ALA172    A         N_762  <--->     GLN168    A          O_694     3.3    29.0
@>     ARG180    A         N_887  <--->     HIS176    A          O_815     3.3    17.0
@>     ILE184    A         N_957  <--->     ARG180    A          O_892     3.3    20.8
@>     VAL377    A        N_3952  <--->     MET373    A         O_3882     3.3    17.5
@>     GLY216    A        N_1501  <--->     ALA213    A         O_1463     3.4    18.2
```

```
@>     THR384    A      OG1_4084  <--->     HIS380    A        O_4007     3.4    28.3
@>     ILE301    A        N_2693  <--->     PRO297    A        O_2637     3.4    30.7
@>     ARG362    A        N_3682  <--->     ASP358    A        O_3626     3.4    14.3
@>     THR337    A        N_3269  <--->     THR333    A        O_3207     3.4     8.2
@>     ALA241    A        N_1922  <--->     THR238    A        O_1879     3.4    39.5
@>     GLU379    A        N_3987  <--->     ARG375    A        O_3918     3.4    33.0
@>     TRP313    A        N_2888  <--->     LYS309    A        O_2824     3.4    22.9
@>     GLU330    A        N_3163  <--->     PRO327    A        O_3119     3.4    15.1
@>     LEU323    A        N_3051  <--->     CYS319    A        O_2989     3.4    34.6
@>     TYR295    A        N_2593  <--->     THR292    A        O_2553     3.5    19.4
@> Number of detected hydrogen bonds: 62.
@> Creating file with dummy atoms
@> struc_homologs/align__addH_model20.pdb
@> 4205 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> Calculating hydrogen bonds.
..
..
```

Analysis of the folder with prepared PDB homologs, including the MSA file generated by `runFoldseek()` function:

```
In [15]: calcSignatureInteractions('struc_homologs', mapping_file='shortlisted_resind.msa')
```

```
@> [INFO] Processing HBs
@> [INFO] Loading mapping file: shortlisted_resind.msa
@> 2158 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> [INFO] Processing PDB files in folder: struc_homologs_MSA
@> [INFO] Processing file 1: struc_homologs_MSA/align__addH_model65.pdb
@> 4126 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     ARG357    A       NE_3612  <--->     VAL352    A        O_3540     2.7    38.9
@>     LEU225    A        N_1656  <--->     GLU221    A        O_1588     2.8    32.6
@>     ALA150    A         N_372  <--->     LEU159    A         O_537     2.8    30.0
@>     ARG357    A        N_3597  <--->     THR353    A        O_3556     2.9    30.8
@>     LEU159    A         N_532  <--->     ALA150    A         O_377     2.9    29.3
@>     LEU149    A         N_353  <--->     ARG137    A         O_165     2.9    15.6
@>     ARG371    A       NE_3854  <--->     LYS365    A        O_3749     2.9    37.3
@>     MET373    A        N_3877  <--->     GLU376    A      OE1_3950     2.9     2.4
@>     TYR338    A        N_3283  <--->     TYR334    A        O_3221     2.9    20.2
@>     GLU239    A        N_1888  <--->     THR235    A        O_1825     2.9    31.3
@>     CYS319    A        N_2984  <--->     LEU315    A        O_2928     2.9    20.3
@>     VAL344    A        N_3404  <--->     ILE341    A        O_3355     2.9    39.6
@>     VAL163    A         N_602  <--->     ASN146    A         O_307     3.0    29.5
@>     ALA160    A         N_551  <--->     CYS210    A        O_1416     3.0    22.2
@>     LEU169    A         N_706  <--->     PHE165    A         O_642     3.0    36.1
@>     GLU321    A        N_3016  <--->     VAL317    A        O_2954     3.0    30.5
@>     LYS224    A        N_1634  <--->     ARG220    A        O_1564     3.0    23.9
@>     HIS380    A        N_4002  <--->     VAL377    A        O_3957     3.0    19.8
@>     VAL317    A        N_2949  <--->     TRP313    A        O_2893     3.0    27.3
@>     TYR246    A        N_1986  <--->     ASN242    A        O_1937     3.0    34.8
@>     ASN242    A        N_1932  <--->     THR238    A        O_1879     3.0    27.4
@>     ILE209    A        N_1392  <--->     GLY198    A        O_1217     3.1    27.2
@>     THR238    A        N_1874  <--->     ALA234    A        O_1815     3.1    32.0
@>     CYS247    A        N_2007  <--->     ALA243    A        O_1951     3.1    36.4
@>     TYR246    A       OH_2005  <--->     ARG189    A        N_1040     3.1    28.4
@>     ALA243    A        N_1946  <--->     GLU239    A        O_1893     3.1    15.4
@>     ALA385    A        N_4090  <--->     PRO381    A        O_4023     3.1    26.6
@>     TYR148    A         N_332  <--->     LEU161    A         O_566     3.1    34.4
@>     SER361    A        N_3671  <--->     ARG357    A        O_3602     3.1    14.6
```

```
@>     LEU296    A        N_2614  <--->     LEU293    A        O_2567     3.1    25.1
@>     ILE360    A        N_3652  <--->     ALA356    A        O_3592     3.1    31.3
@>     LEU315    A        N_2923  <--->     ASP311    A        O_2862     3.1    26.1
@>     GLN223    A        N_1617  <--->     TYR219    A        O_1543     3.1    18.3
@>     LYS250    A        N_2046  <--->     TYR246    A        O_1991     3.1    38.7
@>     GLU336    A        N_3254  <--->     THR333    A      OG1_3210     3.1    27.3
@>     THR235    A        N_1820  <--->     GLN231    A        O_1760     3.1    31.5
@>     SER249    A        N_2035  <--->     SER245    A        O_1980     3.2    13.1
@>     SER314    A        N_2912  <--->     VAL310    A        O_2846     3.2    20.2
@>     LYS250    A       NZ_2064  <--->     HIS187    A        O_1009     3.2    22.6
@>     ASP202    A        N_1276  <--->     ARG205    A        O_1317     3.2    32.9
@>     TYR320    A        N_2995  <--->     GLY316    A        O_2948     3.2    26.2
@>     TYR219    A        N_1538  <--->     PRO259    A        O_2225     3.2    18.1
@>     LEU359    A        N_3633  <--->     GLY355    A        O_3586     3.2     5.7
@>     LEU363    A        N_3706  <--->     LEU359    A        O_3638     3.2    29.4
@>     ALA129    A          N_43  <--->     ASP132    A        OD2_98     3.3    33.5
@>     VAL352    A        N_3535  <--->     PRO349    A        O_3493     3.3    28.8
@>     GLY316    A        N_2942  <--->     LEU312    A        O_2874     3.3    31.9
@>     ALA172    A         N_762  <--->     GLN168    A         O_694     3.3    29.0
@>     ARG180    A         N_887  <--->     HIS176    A         O_815     3.3    17.0
@>     ILE184    A         N_957  <--->     ARG180    A         O_892     3.3    20.8
@>     VAL377    A        N_3952  <--->     MET373    A        O_3882     3.3    17.5
@>     GLY216    A        N_1501  <--->     ALA213    A        O_1463     3.4    18.2
@>     THR384    A      OG1_4084  <--->     HIS380    A        O_4007     3.4    28.3
@>     ILE301    A        N_2693  <--->     PRO297    A        O_2637     3.4    30.7
@>     ARG362    A        N_3682  <--->     ASP358    A        O_3626     3.4    14.3
@>     THR337    A        N_3269  <--->     THR333    A        O_3207     3.4     8.2
@>     ALA241    A        N_1922  <--->     THR238    A        O_1879     3.4    39.5
@>     GLU379    A        N_3987  <--->     ARG375    A        O_3918     3.4    33.0
@>     TRP313    A        N_2888  <--->     LYS309    A        O_2824     3.4    22.9
@>     GLU330    A        N_3163  <--->     PRO327    A        O_3119     3.4    15.1
@>     LEU323    A        N_3051  <--->     CYS319    A        O_2989     3.4    34.6
@>     TYR295    A        N_2593  <--->     THR292    A        O_2553     3.5    19.4
@> Number of detected hydrogen bonds: 62.
@> Creating file with dummy atoms
@> [INFO] Processing file 2: struc_homologs_MSA/align__addH_model20.pdb
@> 4205 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     HIS380    B        N_4081  <--->     GLU376    B        O_4021     2.8    32.3
@>     LEU263    B        N_2274  <--->     LYS271    B        O_2386     2.9    36.8
@>     LEU149    B         N_336  <--->     ARG137    B         O_148     2.9    34.0
@>     ILE253    B        N_2099  <--->     VAL279    B        O_2511     2.9    31.0
@>     ALA385    B        N_4169  <--->     PRO381    B        O_4102     2.9    32.3
@>     LEU240    B        N_1894  <--->     TYR236    B        O_1830     2.9    28.2
@>     CYS247    B        N_1998  <--->     ALA243    B        O_1942     2.9    26.9
@>     TYR320    B        N_3074  <--->     GLY316    B        O_3027     3.0    22.9
@>     VAL252    B        N_2083  <--->     CYS247    B        O_2003     3.0    39.7
@>     SER342    B        N_3448  <--->     TYR338    B        O_3367     3.0    18.9
@>     TYR246    B        N_1977  <--->     ASN242    B        O_1928     3.0    34.7
@>     VAL317    B        N_3028  <--->     TRP313    B        O_2972     3.0    19.8
@>     ALA243    B        N_1937  <--->     GLU239    B        O_1884     3.0    33.7
@>     ARG195    B        N_1130  <--->     GLU211    B      OE2_1427     3.0    31.8
@>     PHE322    B        N_3110  <--->     LEU318    B        O_3049     3.0    21.6
@>     GLU170    B         N_708  <--->     LYS166    B         O_645     3.0    30.4
@>     TYR236    B        N_1825  <--->     ARG232    B        O_1768     3.0    12.3
@>     GLN185    B         N_959  <--->     GLU181    B         O_899     3.0    35.5
@>     SER155    B         N_443  <--->     GLU152    B       OE1_402     3.0    32.8
```

```
@>     THR337    B        N_3348  <--->     THR333    B        O_3286     3.0    22.5
@>     ALA241    B        N_1913  <--->     ILE237    B        O_1851     3.0    12.7
@>     GLU134    B         N_102  <--->     ARG151    B         O_370     3.0    36.4
@>     HIS254    B        N_2118  <--->     ASP311    B      OD2_2947     3.0    19.4
@>     ILE272    B        N_2403  <--->     ASN192    B        O_1083     3.0    32.2
@>     LEU359    B        N_3712  <--->     GLY355    B        O_3665     3.0     5.9
@>     LYS224    B        N_1625  <--->     ARG220    B        O_1555     3.1    39.7
@>     VAL182    B         N_909  <--->     LEU178    B         O_832     3.1    11.8
@>     ARG151    B         N_365  <--->     GLU134    B         O_107     3.1    37.7
@>     ARG362    B        N_3761  <--->     ASP358    B        O_3705     3.1    28.6
@>     THR233    B        N_1787  <--->     ASP229    B        O_1724     3.1    19.5
@>     ARG220    B      NH1_1568  <--->     GLN223    B      OE1_1621     3.1    35.1
@>     ASP358    B        N_3700  <--->     GLU354    B        O_3649     3.1    11.1
@>     LEU169    B         N_689  <--->     PHE165    B         O_625     3.1    18.5
@>     GLU221    B        N_1574  <--->     THR217    B        O_1504     3.2    29.6
@>     TYR338    B        N_3362  <--->     TYR334    B        O_3300     3.2    36.1
@>     LEU215    B        N_1473  <--->     LEU264    B        O_2298     3.2    29.8
@>     GLU379    B        N_4066  <--->     ARG375    B        O_3997     3.2    19.4
@>     LEU296    B        N_2693  <--->     LEU293    B        O_2646     3.2    21.4
@>     ALA172    B         N_745  <--->     GLN168    B         O_677     3.2    34.6
@>     ILE301    B        N_2772  <--->     PRO297    B        O_2716     3.2    17.8
@>     GLY316    B        N_3021  <--->     LEU312    B        O_2953     3.2    31.8
@>     LEU178    B         N_827  <--->     VAL174    B         O_767     3.2    38.9
@>     ARG232    B        N_1763  <--->     ASP229    B      OD1_1729     3.2    29.7
@>     ILE209    B        N_1375  <--->     GLY198    B        O_1200     3.3     9.5
@>     LEU222    B        N_1589  <--->     TYR219    B        O_1534     3.3    29.3
@>     SER249    B        N_2026  <--->     SER245    B        O_1971     3.3    29.7
@>     ARG357    B        N_3676  <--->     THR353    B        O_3635     3.3    39.5
@>     LYS166    B         N_640  <--->     THR204    B        O_1286     3.3    38.8
@>     VAL310    B        N_2920  <--->     ASP307    B        O_2876     3.3     9.5
@>     TRP313    B        N_2967  <--->     LYS309    B        O_2903     3.3    15.1
@>     VAL147    B         N_299  <--->     GLY140    B         O_206     3.4    26.0
@>     TYR219    B        N_1529  <--->     PRO259    B        O_2216     3.4    10.3
@>     HIS254    B      ND1_2128  <--->     ILE257    B        N_2171     3.4    31.5
@>     HIS248    B        N_2009  <--->     SER245    B        O_1971     3.4    33.3
@>     GLN370    B        N_3901  <--->     ASN367    B      ND2_3873     3.4    34.9
@>     ASN386    B        N_4179  <--->     TRP382    B        O_4117     3.5    29.4
@>     LEU323    B        N_3130  <--->     CYS319    B        O_3068     3.5    20.8
@> Number of detected hydrogen bonds: 57.
@> Creating file with dummy atoms
..
..
```

Once the calculations are completed and files with the prefix `'INT_'` are generated, we can look at the clusters for each type of interaction. When we are providing an MSA file for analysis, besides `INT_*.pdb` files, several additional files are generated, such as consensus `txt` files with pairs of residues that are participating in each type of interactions and their count/percentage of occurence among the homolog structures.

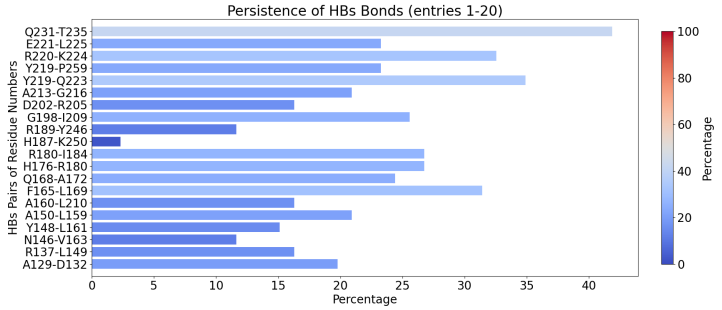
For this example, we obtained six consensus files: `HBs_consensus.txt`, `SBs_consensus.txt`, `RIB_consensus.txt`, `PiStack_consensus.txt`, `PiCat_consensus.txt`, `HPh_consensus.txt`. Disulfide bonds are not present in the protein structure.

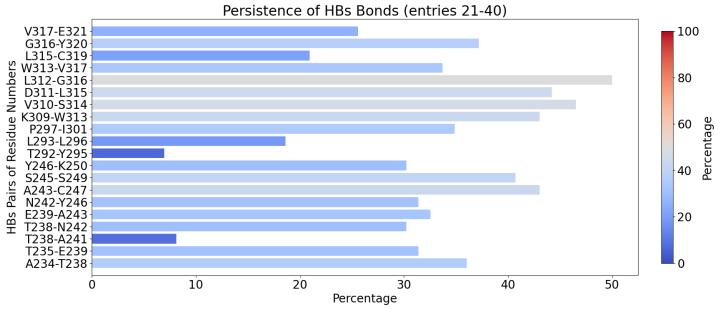
The file `HBs_consensus.txt` content is as follows:

```
Res1 Res2 Count Percentage
A129 D132 17 19.767441860465116
R137 L149 14 16.27906976744186
N146 V163 10 11.627906976744185
Y148 L161 13 15.11627906976744
```

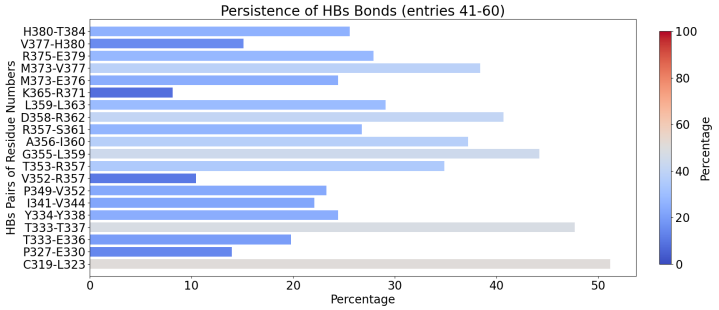
```
A150 L159 18 20.930232558139537
A160 L210 14 16.27906976744186
F165 L169 27 31.3953488372093
Q168 A172 21 24.418604651162788
H176 R180 23 26.744186046511626
R180 I184 23 26.744186046511626
H187 K250 2 2.3255813953488373
R189 Y246 10 11.627906976744185
G198 I209 22 25.581395348837212
D202 R205 14 16.27906976744186
A213 G216 18 20.930232558139537
Y219 Q223 30 34.883720930232556
Y219 P259 20 23.25581395348837
R220 K224 28 32.55813953488372
E221 L225 20 23.25581395348837
Q231 T235 36 41.86046511627907
A234 T238 31 36.04651162790697
T235 E239 27 31.3953488372093
T238 A241 7 8.13953488372093
T238 N242 26 30.23255813953488
E239 A243 28 32.55813953488372
N242 Y246 27 31.3953488372093
A243 C247 37 43.02325581395349
S245 S249 35 40.69767441860465
Y246 K250 26 30.23255813953488
..
..
```

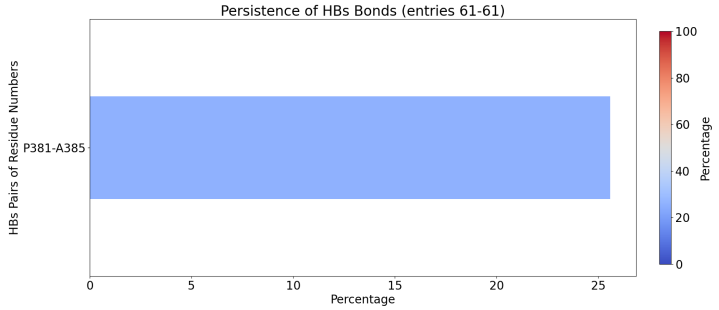
This content is also displayed on the plot in `PNG` format that is saved in the folder. If there are a lot of results, several plots will be created, as exemplified by hydrogen bonds for which we identified 61 pairs of residues.

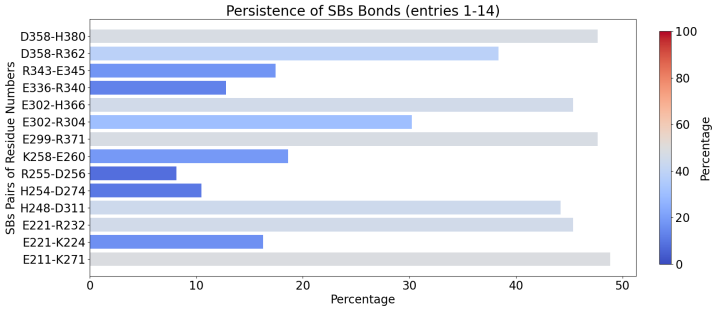




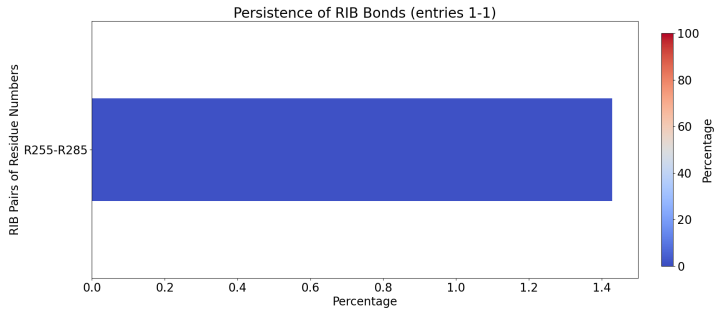
For the salt bridges, we obtained the following plot:


Persistence of HBs Bonds (entries 41-60)
HBs Pairs of Residue Numbers
H380-T384
V377-H380
R375-E379
M373-V377
M373-E376
K365-R371
L359-L363
D358-R362
R357-S361
A356-I360
G355-L359
T353-R357
V352-R357
P349-V352
I341-V344
Y334-Y338
T333-T337
T333-E336
P327-E330
C319-L323
0
10
20
30
40
50
Percentage
100
80
60
40
20
0
Percentage

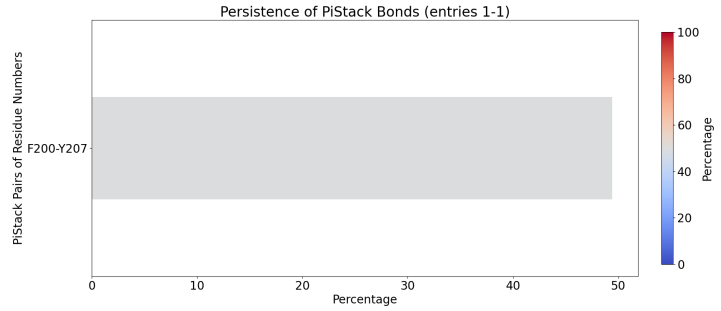

Persistence of HBs Bonds (entries 61-61)
HBs Pairs of Residue Numbers
P381-A385
0
5
10
15
20
25
Percentage
100
80
60
40
20
0
Percentage


Persistence of SBs Bonds (entries 1-14)
SBs Pairs of Residue Numbers
D358-H380
D358-R362
R343-E345
E336-R340
E302-H366
E302-R304
E299-R371
K258-E260
R255-D256
H254-D274
H248-D311
E221-R232
E221-K224
E211-K271
0
10
20
30
40
50
Percentage
100
80
60
40
20
0
Percentage

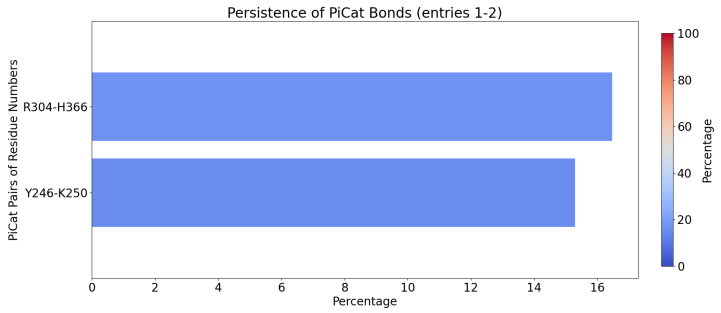
For the repulsive ionic bonding, we obtained the following plot:



For the pi-stacking interactions, we obtained the following plot:



For the pi-cation interactions, we obtained the following plot:

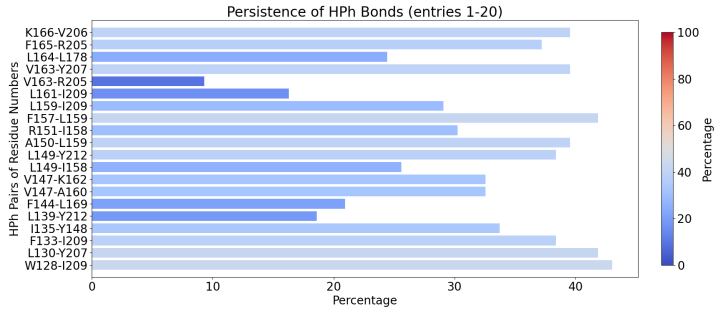


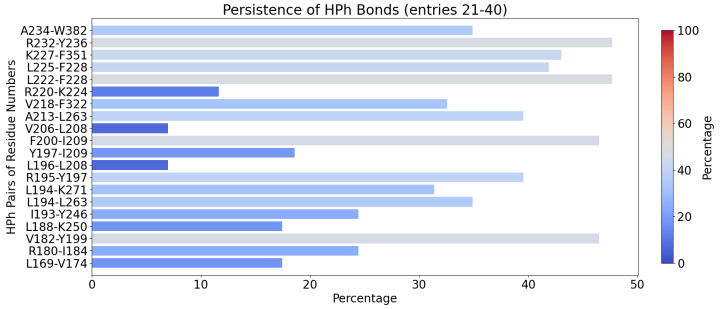
For the hydrophobic interactions, we obtained the following plots:

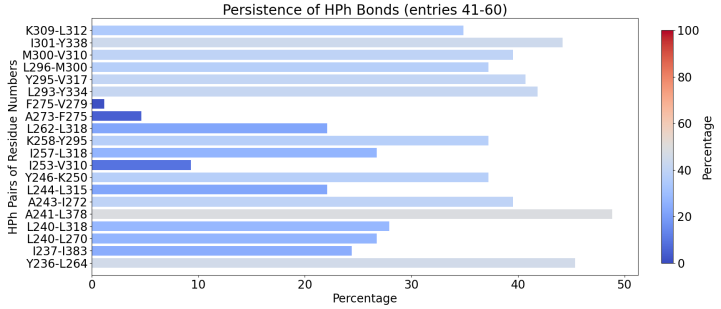
Further, to compute the fingerprint interactions, use the corresponding prefix. For hydrogen bonds is `INT_HBs_`:

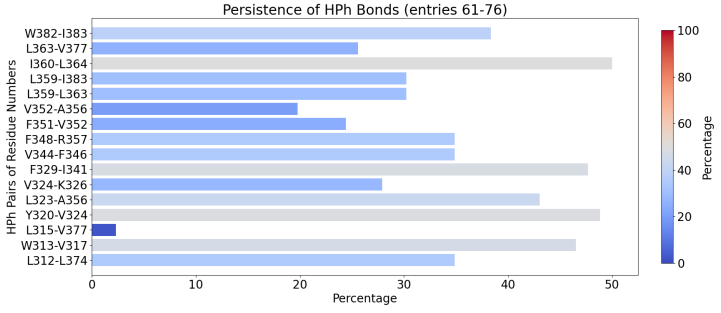
```
In [16]: findClusterCenters('INT_HBs_*.pdb', selection = 'resname DUM')
```

```
@> 4338 atoms and 1 coordinate set(s) were parsed in 0.12s.
@> 4230 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4231 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4328 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4284 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4365 atoms and 1 coordinate set(s) were parsed in 0.05s.
..
@> 4062 atoms and 1 coordinate set(s) were parsed in 0.04s.
```


Persistence of HPh Bonds (entries 1-20)
K166-V206
F165-R205
L164-L178
V163-Y207
V163-R205
L161-I209
L159-I209
F157-L159
R151-I158
A150-L159
L149-Y212
L149-I158
V147-K162
V147-A160
F144-L169
L139-Y212
I135-Y148
F133-I209
L130-Y207
W128-I209
HPh Pairs of Residue Numbers
0
10
20
30
40
Percentage
100
80
60
40
20
0
Percentage

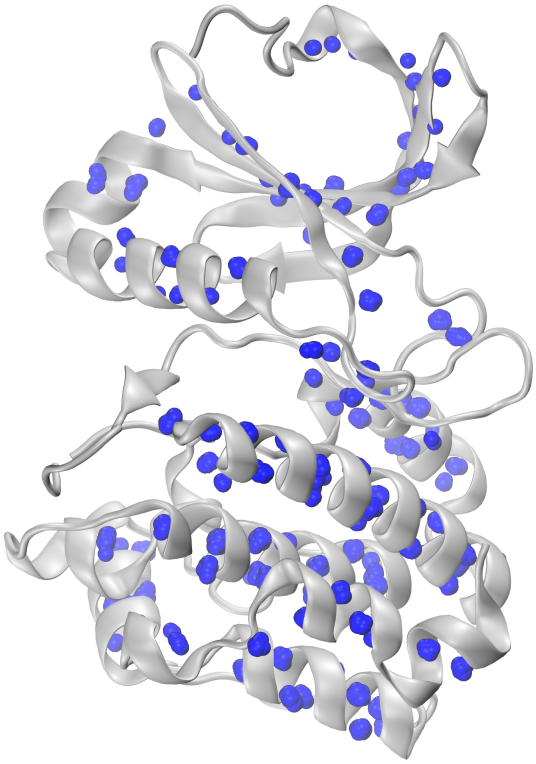

Persistence of HPh Bonds (entries 21-40)
A234-W382
R232-Y236
K227-F351
L225-F228
L222-F228
R220-K224
V218-F322
A213-L263
V206-L208
F200-I209
Y197-I209
L196-L208
R195-Y197
L194-K271
L194-L263
I193-Y246
L188-K250
V182-Y199
R180-I184
L169-V174
HPh Pairs of Residue Numbers
0
10
20
30
40
50
Percentage
100
80
60
40
20
0
Percentage


Persistence of HPh Bonds (entries 41-60)
K309-L312
I301-Y338
M300-V310
L296-M300
Y295-V317
L293-Y334
F275-V279
A273-F275
L262-L318
K258-Y295
I257-L318
I253-V310
Y246-K250
L244-L315
A243-I272
A241-L378
L240-L318
L240-L270
I237-I383
Y236-L264
HPh Pairs of Residue Numbers
0
10
20
30
40
50
Percentage
100
80
60
40
20
0
Percentage


Persistence of HPh Bonds (entries 61-76)
W382-I383
L363-V377
I360-L364
L359-I383
L359-L363
V352-A356
F351-V352
F348-R357
V344-F346
F329-I341
V324-K326
L323-A356
Y320-V324
L315-V377
W313-V317
L312-L374
HPh Pairs of Residue Numbers
0
10
20
30
40
50
Percentage
100
80
60
40
20
0
Percentage

```
@> 4389 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Results are saved in clusters_INT_HBs_.pdb.
```

When we visualize `clusters_INT_HBs_.pdb` in the graphical program with protein structure, we will see:



To compute fingerprint interactions of salt bridges, use the prefix `INT_SBs_`:

```
In [17]: findClusterCenters('INT_SBs_*.pdb', selection = 'resname DUM')
```

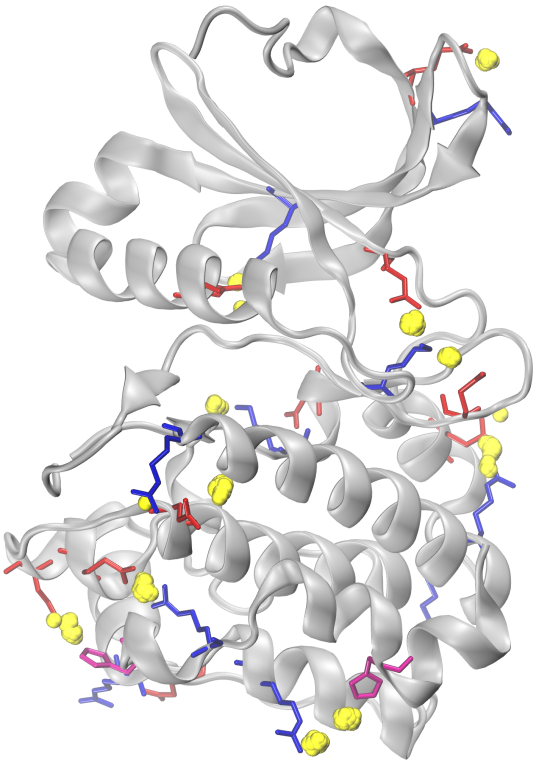
```
@> 4305 atoms and 1 coordinate set(s) were parsed in 0.12s.
@> 4191 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4193 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4280 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4239 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4187 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4059 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4214 atoms and 1 coordinate set(s) were parsed in 0.05s
..
@> 4021 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4306 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Results are saved in clusters_INT_SBs_.pdb.
```

When we visualize `clusters_INT_SBs_.pdb` in the graphical program with protein structure, we will see:

To compute the fingerprint of pi-stacking interactions, use the prefix `INT_PiCat_`:

```
In [18]: findClusterCenters('INT_PiCat_*.pdb', selection = 'resname DUM')
```

```
@> 4291 atoms and 1 coordinate set(s) were parsed in 0.12s.
@> 4180 atoms and 1 coordinate set(s) were parsed in 0.05s.
```



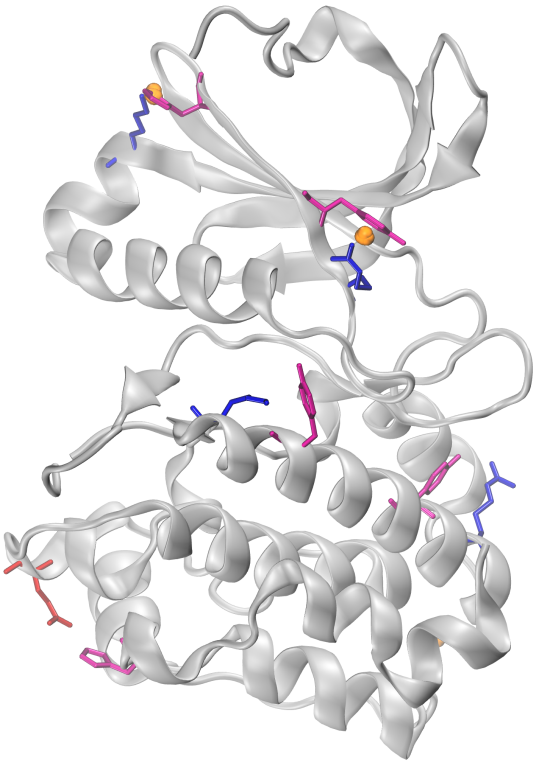
```
@> 4185 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4268 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4224 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4174 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4048 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4200 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4225 atoms and 1 coordinate set(s) were parsed in 0.06s.
@> 4336 atoms and 1 coordinate set(s) were parsed in 0.05s.
..
..
@> 4112 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4191 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4010 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4127 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4009 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Results are saved in clusters_INT_PiCat_.pdb.
```

When we visualize `clusters_INT_PiCat_.pdb` in the graphical program with protein structure, we will see:

To compute the fingerprint of pi-stacking interactions, use the prefix `INT_PiStack_`:

```
In [19]: findClusterCenters('INT_PiStack_*.pdb', selection = 'resname DUM')
```

```
@> 4291 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4178 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4182 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4267 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4223 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4172 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4047 atoms and 1 coordinate set(s) were parsed in 0.04s.
```



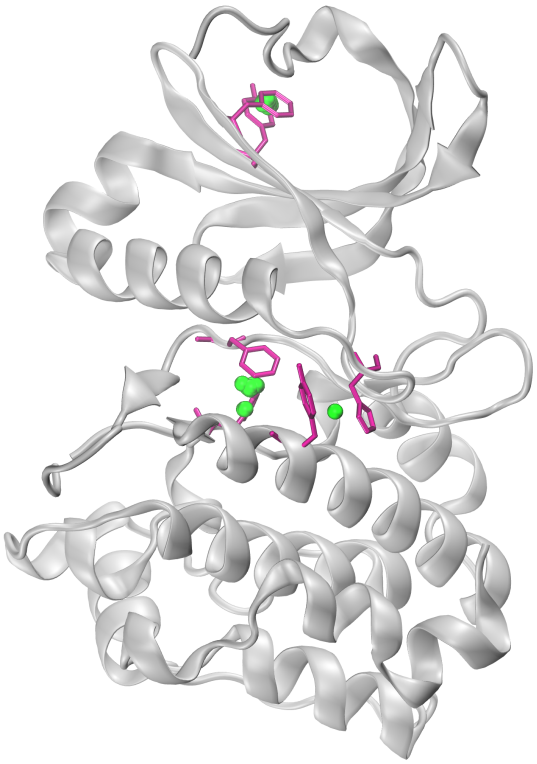
```
@> 4200 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4223 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4335 atoms and 1 coordinate set(s) were parsed in 0.05s.
..
..
@> 4104 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4114 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4192 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4009 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4129 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4008 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4291 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Results are saved in clusters_INT_PiStack_.pdb.
```

When we visualize `clusters_INT_PiStack_.pdb` in the graphical program with protein structure, we will see:

To compute fingerprint interactions of repulsive ionic bonding, use the prefix `INT_RIB_`:

```
In [20]: findClusterCenters('INT_RIB_*.pdb', selection = 'resname DUM')
```

```
@> 4291 atoms and 1 coordinate set(s) were parsed in 0.12s.
@> 4177 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4182 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4266 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4222 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4199 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4334 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4206 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4217 atoms and 1 coordinate set(s) were parsed in 0.05s.
```



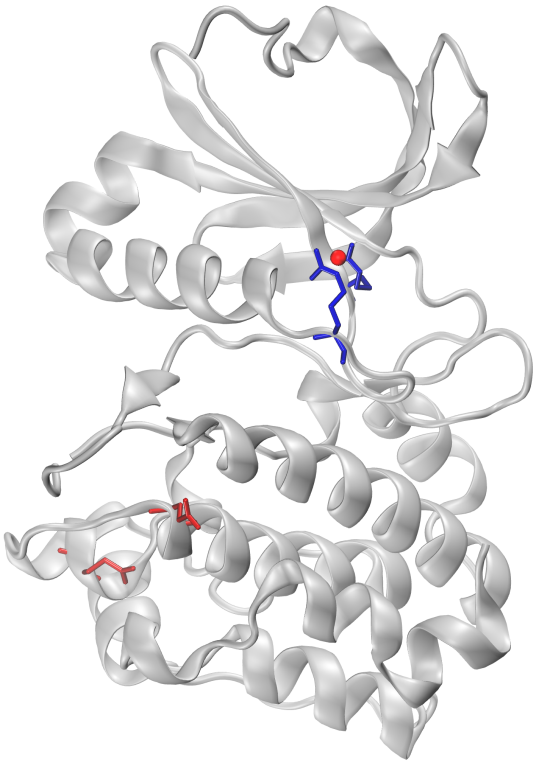
```
..
..
@> 4204 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4103 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4112 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4190 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4008 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4290 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Results are saved in clusters_INT_RIB_.pdb.
```

When we visualize `clusters_INT_RIB_.pdb` in the graphical program with protein structure, we will see:

To compute the fingerprint of hydrophobic interactions, use the prefix `INT_HPh_`:

```
In [21]: findClusterCenters('INT_HPh_*.pdb', selection = 'resname DUM')
```

```
@> 4371 atoms and 1 coordinate set(s) were parsed in 0.12s.
@> 4253 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4257 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4346 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4304 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4249 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4124 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4280 atoms and 1 coordinate set(s) were parsed in 0.05s.
@> 4298 atoms and 1 coordinate set(s) were parsed in 0.05s.
..
..
@> 4195 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4265 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4085 atoms and 1 coordinate set(s) were parsed in 0.04s.
```



```
@> 4210 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4087 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> 4365 atoms and 1 coordinate set(s) were parsed in 0.04s.
@> Results are saved in clusters_INT_HPh_.pdb.
```

When we visualize `clusters_INT_HPh_.pdb` in the graphical program with protein structure, we will see:

If we compare BLAST and Foldseek results, we can see that, in this case, BLAST detected more conserved interactions. However, the results for Foldseek or Dali would look differently if we used a full database with default parameters. It is important, however, to know that some of the methods might be better than others, and all depends on the protein we are choosing, their sequence identity, and 3D structure similarity toward homologs.

Acknowledgments

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[17] http://www.nih.gov/
[18] http://mmbios.org/