Create_interchain_hbond_tables

November 9, 2017

```
In [1]: %time import pandas as pd

CPU times: user 532 ms, sys: 160 ms, total: 692 ms
Wall time: 645 ms


In [2]: %%time
        pd.set_option('display.max_rows', 10)
        pd.set_option('display.max_columns', 100)

CPU times: user 0 ns, sys: 0 ns, total: 0 ns
Wall time: 92.7 µs


In [3]: %%time
        phase1 = pd.read_csv("../TT_Phases_PDB/rRNA_rPro/LSU_Phase1_rRNA_all_rPro.contacts", sep
                             names=['Atom 1','Atom 2','Clash','Covalent','VdW Clash','VdW','Prox
                                    'Hydrogen Bond','Weak Hydrogen Bond','Halogen Bond','Ionic',
                                    'Metal Complex','Aromatic','Hydrophobic','Carbonyl','Polar',
                                    'Weak Polar','Interacting entities'])

CPU times: user 244 ms, sys: 32 ms, total: 276 ms
Wall time: 482 ms


In [4]: %time phase1

CPU times: user 0 ns, sys: 0 ns, total: 0 ns
Wall time: 12.2 µs


Out[4]:           Atom 1    Atom 2  Clash  Covalent  VdW Clash  VdW  Proxima  \
        0         F/16/C   F/18/CA      0         0          0    0        1
        1         F/16/O   F/18/CA      0         0          0    0        1
        2         F/17/C    F/19/N      0         0          0    0        1
        3         F/11/O    F/17/O      0         0          0    0        1
        4         F/11/O   F/18/CA      0         0          0    0        1
        ...          ...       ...    ...       ...        ...  ...      ...
        135040  4/65/OD2  4/502/MG      0         0          0    0        1
```

```
135041   4/65/CG  4/502/MG      0         0          0    0        1
135042    4/65/O  4/502/MG      0         0          0    0        1
135043    4/67/O    4/65/O      0         0          0    0        1
135044    4/67/C    4/65/C      0         0          0    0        1

        Hydrogen Bond  Weak Hydrogen Bond  Halogen Bond  Ionic  Metal Complex  \
0                   0                   0             0      0              0
1                   0                   0             0      0              0
2                   0                   0             0      0              0
3                   0                   0             0      0              0
4                   0                   0             0      0              0
...               ...                 ...           ...    ...            ...
135040              0                   0             0      0              0
135041              0                   0             0      0              0
135042              0                   0             0      0              0
135043              0                   0             0      0              0
135044              0                   0             0      0              0

        Aromatic  Hydrophobic  Carbonyl  Polar  Weak Polar  \
0              0            0         0      0           0
1              0            0         0      0           0
2              0            0         0      0           0
3              0            0         0      0           0
4              0            0         0      0           0
...          ...          ...       ...    ...         ...
135040         0            0         0      0           0
135041         0            0         0      0           0
135042         0            0         0      0           0
135043         0            0         0      0           0
135044         0            0         0      0           0

       Interacting entities
0           INTRA_SELECTION
1           INTRA_SELECTION
2           INTRA_SELECTION
3           INTRA_SELECTION
4           INTRA_SELECTION
...                     ...
135040      INTRA_SELECTION
135041      INTRA_SELECTION
135042      INTRA_SELECTION
135043      INTRA_SELECTION
135044      INTRA_SELECTION

[135045 rows x 18 columns]
```

```
In [5]: %time phase1[['chain1', 'resnum1', 'atom1']] = phase1['Atom 1'].str.split('/', expand=Tr
```

```
CPU times: user 500 ms, sys: 20 ms, total: 520 ms
```

```
Wall time: 537 ms
```

```
In [6]: phase1[['chain2', 'resnum2', 'atom2']] = phase1['Atom 2'].str.split('/', expand=True)
```

```
In [7]: phase1_hbonds = phase1.loc[phase1['Hydrogen Bond'] == 1]
```

```
In [8]: phase1_hbonds
```

Out[8]:

	Atom 1	Atom 2	Clash	Covalent	VdW Clash	VdW	Proxima	\
11	F/11/N	F/18/O	0	0	0	1	0	
103	F/152/OE2	F/122/NZ	0	0	0	0	1	
133	P/2/NZ	P/4/OG	0	0	0	0	1	
220	F/202/O	F/206/N	0	0	0	0	1	
268	F/204/O	F/207/N	0	0	0	0	1	
...	...	...	...	...	...	...	...	
134745	Z/139/N	Z/103/O	0	0	1	0	0	
134750	Z/137/O	Z/103/N	0	0	1	0	0	
134914	Z/144/O	Z/109/N	0	0	1	0	0	
134944	Z/141/N	Z/105/O	0	0	1	0	0	
134998	4/65/O	4/67/N	0	0	0	1	0	

	Hydrogen Bond	Weak Hydrogen Bond	Halogen Bond	Ionic	Metal Complex	\
11	1	0	0	0	0	
103	1	0	0	1	0	
133	1	0	0	0	0	
220	1	0	0	0	0	
268	1	0	0	0	0	
...	...	...	...	...	...	
134745	1	0	0	0	0	
134750	1	0	0	0	0	
134914	1	0	0	0	0	
134944	1	0	0	0	0	
134998	1	0	0	0	0	

	Aromatic	Hydrophobic	Carbonyl	Polar	Weak Polar	\
11	0	0	0	1	0	
103	0	0	0	1	0	
133	0	0	0	0	0	
220	0	0	0	1	0	
268	0	0	0	1	0	
...	...	...	...	...	...	
134745	0	0	0	1	0	
134750	0	0	0	1	0	
134914	0	0	0	1	0	
134944	0	0	0	1	0	
134998	0	0	0	1	0	

	Interacting entities	chain1	resnum1	atom1	chain2	resnum2	atom2

```
11          INTRA_SELECTION      F      11     N      F      18     O
103         INTRA_SELECTION      F     152   OE2      F     122    NZ
133         INTRA_SELECTION      P       2    NZ      P       4    OG
220         INTRA_SELECTION      F     202     O      F     206     N
268         INTRA_SELECTION      F     204     O      F     207     N
...                     ...    ...     ...   ...    ...     ...   ...
134745      INTRA_SELECTION      Z     139     N      Z     103     O
134750      INTRA_SELECTION      Z     137     O      Z     103     N
134914      INTRA_SELECTION      Z     144     O      Z     109     N
134944      INTRA_SELECTION      Z     141     N      Z     105     O
134998      INTRA_SELECTION      4      65     O      4      67     N

[3362 rows x 24 columns]
```

In [9]:
```
phase1_interchain_hbonds_phase1 = phase1_hbonds.query('chain1 != chain2')
```

In [10]:
```
phase1_interchain_hbonds_phase1
```

Out[10]:

```
            Atom 1      Atom 2  Clash  Covalent  VdW Clash  VdW  Proxima  \
345      F/117/NH2       P/1/O      0         0          1    0        0
2089    A/2444/OP1    F/67/NE2      0         0          1    0        0
2125      F/74/NH2  A/2445/OP1      0         0          1    0        0
2959    A/2075/OP1   D/244/NH2      0         0          0    0        1
4398         X/5/O    2/36/NH2      0         0          1    0        0
...            ...         ...    ...       ...        ...  ...      ...
132817   Q/119/NH2  A/2468/OP1      0         0          1    0        0
132918     Q/133/O    Z/81/NH1      0         0          0    0        1
132971    Z/49/NH2   Q/135/OD2      0         0          1    0        0
133113    Q/31/OD1   Z/122/NH2      0         0          0    0        1
133121    Z/81/NH1   Q/138/OD2      0         0          1    0        0

         Hydrogen Bond  Weak Hydrogen Bond  Halogen Bond  Ionic  Metal Complex  \
345                  1                   0             0      0              0
2089                 1                   0             0      0              0
2125                 1                   0             0      1              0
2959                 1                   0             0      1              0
4398                 1                   0             0      0              0
...                ...                 ...           ...    ...            ...
132817               1                   0             0      1              0
132918               1                   0             0      0              0
132971               1                   0             0      1              0
133113               1                   0             0      1              0
133121               1                   0             0      1              0

         Aromatic  Hydrophobic  Carbonyl  Polar  Weak Polar  \
345             0            0         0      1           0
2089            0            0         0      1           0
2125            0            0         0      1           0
```

```
2959          0            0         0      1           0
4398          0            0         0      1           0
...         ...          ...       ...    ...         ...
132817        0            0         0      1           0
132918        0            0         0      1           0
132971        0            0         0      1           0
133113        0            0         0      1           0
133121        0            0         0      1           0
```

	Interacting entities	chain1	resnum1	atom1	chain2	resnum2	atom2
345	INTRA_SELECTION	F	117	NH2	P	1	O
2089	INTRA_SELECTION	A	2444	OP1	F	67	NE2
2125	INTRA_SELECTION	F	74	NH2	A	2445	OP1
2959	INTRA_SELECTION	A	2075	OP1	D	244	NH2
4398	INTRA_SELECTION	X	5	O	2	36	NH2
...	...	...	...	...	...	...	...
132817	INTRA_SELECTION	Q	119	NH2	A	2468	OP1
132918	INTRA_SELECTION	Q	133	O	Z	81	NH1
132971	INTRA_SELECTION	Z	49	NH2	Q	135	OD2
133113	INTRA_SELECTION	Q	31	OD1	Z	122	NH2
133121	INTRA_SELECTION	Z	81	NH1	Q	138	OD2

```
[123 rows x 24 columns]
```

In [ ]: