rna-tools documentation

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USER DOCUMENTATION

rna-tools: a toolbox to analyze structures and simulations of RNA

The code of the project can be found at GitHub https://github.com/mmagnus/rna-tools.

This documentation can be found at http://rna-tools.rtfd.io.

The PDF version of documentation can be found at here.

If something does not work for you, please make an issue, using https://github.com/mmagnus/rna-tools/issues.

CHAPTER

ONE

INSTALL

This guide assumes you already have python and pip installed.

To install pytube, run the following command in your terminal:

```
$ pip install rna-tools
```

1.1 Get the Source Code

rna-toos is actively developed on GitHub, where the source is available:

You can either clone the public repository:

```
$ git clone http://github.com/mmagnus/rna-tools.git
$ cd rna-tools && pip install -e .
```

or (to install in current ./src/):

```
pip install -e git+http://github.com/mmagnus/rna-tools.git#egg=rna-tools
```

CHAPTER

TWO

QUICKSTART

This guide will walk you through the basic usage of rna-tools.

Let's get started with some examples.

2.1 fetch a structure from the PDB database

Example:

```
$ rna_pdb_tools.py --fetch 1xjr
downloading...1xjr ok
```

2.2 fetch a biologicaly assembly

Example:

```
$ rna_pdb_tools.py --fetch-ba 1xjr
downloading...1xjr_ba.pdb ok
```

or over a list of pdb ids in a text file:

```
$ cat data/pdb_ids.txt
1y26
1fir

$ while read p; do rna_pdb_tools.py --fetch-ba $p; done < data/pdb_ids.txt
downloading...1y26_ba.pdb ok
downloading...1fir_ba.pdb ok

$ ls *.pdb
1fir_ba.pdb 1y26_ba.pdb
```

2.3 get sequences of a bunch of PDB files

Example:

```
$ rna_pdb_tools.py --get-seq *.pdb
# 1xjr
> A:1-47
GGAGUUCACCGAGGCCACGCGGAGUACGAUCGAGGGUACAGUGAAUU
# 6TNA
> A:1-76
GCGGAUUUAgCUCAGuuGGGAGAGCgCCAGAcUgAAgAucUGGAGgUCcUGUGuuCGaUCCACAGAAUUCGCACCA
# rp2_bujnicki_1_rpr
> A:1-15
CCGGAGGAACUACUG
> B:1-10
CCGGCAGCCU
> C:1-15
CCGGAGGAACUACUG
> D:1-10
CCGGCAGCCU
> E:1-15
CCGGAGGAACUACUG
> F:1-10
CCGGCAGCCU
> G:1-15
CCGGAGGAACUACUG
> H:1-10
CCGGCAGCCU
```

in some more fancy way ;-)

```
$ rna_pdb_tools.py --get-seq \
          --oneline 3_bujnicki_1_rpr* \
          --color-seq --compact
```

```
(py37) [mx] rp03$ git:(master) ✗ rna_pdb_toolsx.py --get-seq --oneline 3_bujnicki_1_rpr* --color-seq --compact
CUCUGGGGGGGGCCGGUUUUCGGGGUCGGCCGGGGGGGGCGGCUCUGGCGGCUUGGCGGGGUGGCUCUCGGGGCGGGGCGGGG # A:1-84 # 3_bujnicki_1_rpr
CUCUGGGGGGGGCCGGUUUUCGGGGUCGGCCGGGGGGGGCGGCUCUGGCGGGGCGGCGGGGUGGCUCUCGGGGCGGGGCGGGG # A:1-84 # 3_bujnicki_1_rpr_mut
```

2.4 get secondary structures of your PDB files

Python parser to 3dna <http://x3dna.org/>.

Installation:

```
# install the code from http://forum.x3dna.org/downloads/3dna-download/
Create a copy of the rna_x3dna_config_local_sample.py (remove "_sample") present in rna-
↪tools/rna_tools/tools/rna_x3dna folder.
Edit this line :
BINARY_PATH = <path to your x3dna-dssr file>
matching the path with the path of your x3dna-dssr file.
e.g. in my case: BINARY_PATH = ~/bin/x3dna-dssr.bin
```

For one structure you can run this script as:

```
[mm] py3dna$ git:(master)  ./rna_x3dna.py test_data/1xjr.pdb
test_data/1xjr.pdb
>1xjr nts=47 [1xjr] -- secondary structure derived by DSSR
gGAGUUCACCGAGGCCACGCGGAGUACGAUCGAGGGUACAGUGAAUU
..(((((((...((((.((((.....))..))..))..))).).)))))))
```

For multiple structures in the folder, run the script like this:

```
[mm] py3dna$ git:(master)  ./rna_x3dna.py test_data/*
test_data/1xjr.pdb
>1xjr nts=47 [1xjr] -- secondary structure derived by DSSR
gGAGUUCACCGAGGCCACGCGGAGUACGAUCGAGGGUACAGUGAAUU
..(((((((...((((.((((.....))..))..))..))).).)))))))
test_data/6TNA.pdb
>6TNA nts=76 [6TNA] -- secondary structure derived by DSSR
GCGGAUUUAgCUCAGuuGGGAGAGCgCCAGAcUgAAgAPcUGGAGgUCcUGUGtPCGaUCCACAGAAUUCGCACCA
(((((((..((((.....[..)))).((((.........)))).....(((((..].....)))))))))))....
test_data/rp2_bujnicki_1_rpr.pdb
>rp2_bujnicki_1_rpr nts=100 [rp2_bujnicki_1_rpr] -- secondary structure derived by DSSR
CCGGAGGAACUACUG&CCGGCAGCCU&CCGGAGGAACUACUG&CCGGCAGCCU&CCGGAGGAACUACUG&CCGGCAGCCU&
↪CCGGAGGAACUACUG&CCGGCAGCCU
[[[[(((.....(((&{{{{))))))&(((((((.....(.(&]]]]).))))&[[[[[[......[[[&))))]]].]]&}}}}(((.
↪....(((&]]]])))))))
```

Warning: This script should not be used in this given form with Parallel because it process output files from x3dna that are named always in the same way, e.g. dssr-torsions.txt. #TODO

class rna_tools.tools.rna_x3dna.rna_x3dna.**x3DNA**(*pdbfn*, *show_log=False*)

Atributes:

curr_fn report

get_ion_water_report()

@todo File name: /tmp/tmp0pdNHS

no. of DNA/RNA chains: 0 [] no. of nucleotides: 174 no. of waters: 793 no. of metals: 33 [Na=29, Mg=1, K=3]

get_modifications()

Run find_pair to find modifications.

get_secstruc()

Get secondary structure.

get_seq()

Get sequence.

Somehow 1bzt_1 x3dna UCAGACUUUUAAPCUGA, what is P? P -> u

get_torsions(*outfn*) → str

Get torsion angles into 'torsion.csv' file:

nt,id,res,alpha,beta,gamma,delta,epsilon,zeta,e-z,chi,phase-angle,sugar-type,ssZp,Dp,splay,bpseq
1,g,A.GTP1,nan,nan,142.1,89.5,-131.0,-78.3,-53(BI),-178.2(anti),358.6(C2'-exo),~C3'-endo,4.68,4.68,29.98,0 2,G,A.G2,-75.8,-167.0,57.2,79.5,-143.4,-69.7,-74(BI),-169.2(anti),5.8(C3'-endo),~C3'-endo,4.68,4.76,25.61,0

run_x3dna(*show_log=False*, *verbose=False*)

exception rna_tools.tools.rna_x3dna.rna_x3dna.**x3DNAMissingFile**

2.5 delete a part of of your structure

Examples:

```
$ for i in *pdb; do rna_pdb_tools.py --delete A:46-56 $i > ../rpr_rm_loop/$i ; done
```

go over all files in the current directory, remove a fragment of chain A, residues between 46-56 (including them) and save outputs to in the folder *rpr_rm_loops*.

2.6 get numbering of your structure and rename chains

Rename chain B in structure 4_das_1_rpr.pdb:

```
$ rna_pdb_tools.py --get-seq  4_das_1_rpr.pdb
> 4_das_1_rpr.pdb B:1-126
GGCUUAUCAAGAGAGGUGGAGGGACUGGCCCGAUGAAACCCGGCAACCACUAGUCUAGCGUCAGCUUCGGCUGACGCUAGGCUAGUGGUGCCAAUUCCUGCAG
$ rna_pdb_tools.py --edit 'B:1-126>A:1-126' 4_das_1_rpr.pdb > 4_das_1_rpr2.pdb
$ rna_pdb_tools.py --get-seq  4_das_1_rpr2.pdb
> 4_das_1_rpr2.pdb A:1-126
GGCUUAUCAAGAGAGGUGGAGGGACUGGCCCGAUGAAACCCGGCAACCACUAGUCUAGCGUCAGCUUCGGCUGACGCUAGGCUAGUGGUGCCAAUUCCUGCAG
```

2.7 edit your structure (rename chain)

Examples:

```
$ rna_pdb_tools.py --edit 'A:3-21>A:1-19' 1f27_clean.pdb > 1f27_clean_A1-19.pdb
```

or even:

```
$ rna_pdb_tools.py --edit 'A:3-21>A:1-19,B:22-32>B:20-30' 1f27_clean.pdb > 1f27_clean_
↪renumb.pdb
```

or even, even, do rename X chain to A only for Chen's pdb structures in the folder, in place (so don't create a new file):

```
$ for i in *Chen*; do rna_pdb_tools.py --edit 'X:1-125>A:1-125' $i > ${i}_temp; mv ${i}_
↪temp ${i}; done
# do only edit for Chen's pdb structures, in place.
```

2.8 extract part of your structure

Example:

```
$ rna_pdb_tools.py --extract A:1-4 13_Bujnicki_1_rpr.pdb
REMARK 250 Model edited with rna-tools
REMARK 250  ver 3.1.14
REMARK 250  https://github.com/mmagnus/rna-tools
REMARK 250  Sat May 23 14:54:05 2020
HEADER extract A:1-4
ATOM      1  P     G A   1     -16.883 -12.441   8.021  1.00  0.00           P
ATOM      2  OP1   G A   1     -15.777 -12.225   8.969  1.00  0.00           O
ATOM      3  OP2   G A   1     -16.752 -11.535   6.892  1.00  0.00           O
ATOM      4  O5'   G A   1     -16.882 -13.822   7.219  1.00  0.00           O
ATOM      5  C5'   G A   1     -16.092 -13.871   6.013  1.00  0.00           C
ATOM      6  C4'   G A   1     -16.314 -15.160   5.206  1.00  0.00           C
ATOM      7  O4'   G A   1     -17.723 -14.932   4.905  1.00  0.00           O
ATOM      8  C3'   G A   1     -15.788 -15.216   3.752  1.00  0.00           C
ATOM      9  O3'   G A   1     -14.461 -15.860   3.764  1.00  0.00           O
ATOM     10  C2'   G A   1     -16.841 -15.946   2.969  1.00  0.00           C
(...)
ATOM     84  O2    U A   4     -14.553  -5.285  -7.938  1.00  0.00           O
ATOM     85  N3    U A   4     -14.077  -5.583  -5.727  1.00  0.00           N
ATOM     86  C4    U A   4     -13.451  -6.130  -4.622  1.00  0.00           C
ATOM     87  O4    U A   4     -13.706  -5.737  -3.486  1.00  0.00           O
ATOM     88  C5    U A   4     -12.494  -7.167  -4.998  1.00  0.00           C
ATOM     89  C6    U A   4     -12.318  -7.489  -6.300  1.00  0.00           C
```

2.9 find missing atoms in my structure

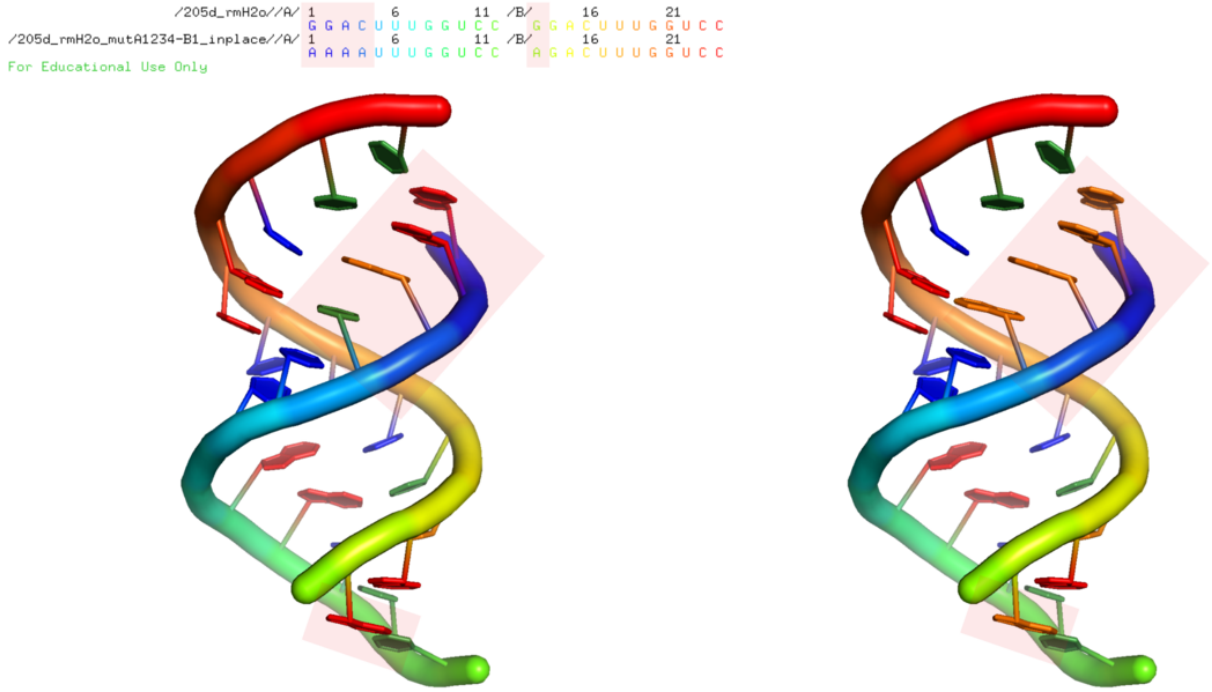
Run:

```
$ rna_pdb_tools.py --get-rnapuzzle-ready input/1_das_1_rpr_fixed.pdb
HEADER Generated with rna-pdb-tools
HEADER ver 91ed4f8-dirty
HEADER https://github.com/mmagnus/rna-pdb-tools
HEADER Sun Mar  5 10:58:07 2017
REMARK 000 Missing atoms:
REMARK 000  + P B <Residue C het=  resseq=1 icode= > residue # 1
REMARK 000  + OP1 B <Residue C het=  resseq=1 icode= > residue # 1
REMARK 000  + OP2 B <Residue C het=  resseq=1 icode= > residue # 1
REMARK 000  + O5' B <Residue C het=  resseq=1 icode= > residue # 1
ATOM      1  P     C A   1     -16.936  -3.789  68.770  1.00 11.89           P
ATOM      2  OP1   C A   1     -17.105  -3.675  67.302  1.00 14.35           O
ATOM      3  OP2   C A   1     -15.666  -4.265  69.342  1.00 12.68           O
...
```

2.10 mutate residues

For example, to replace the first four residues of chain A into adenines and 13th A of chain B, run:

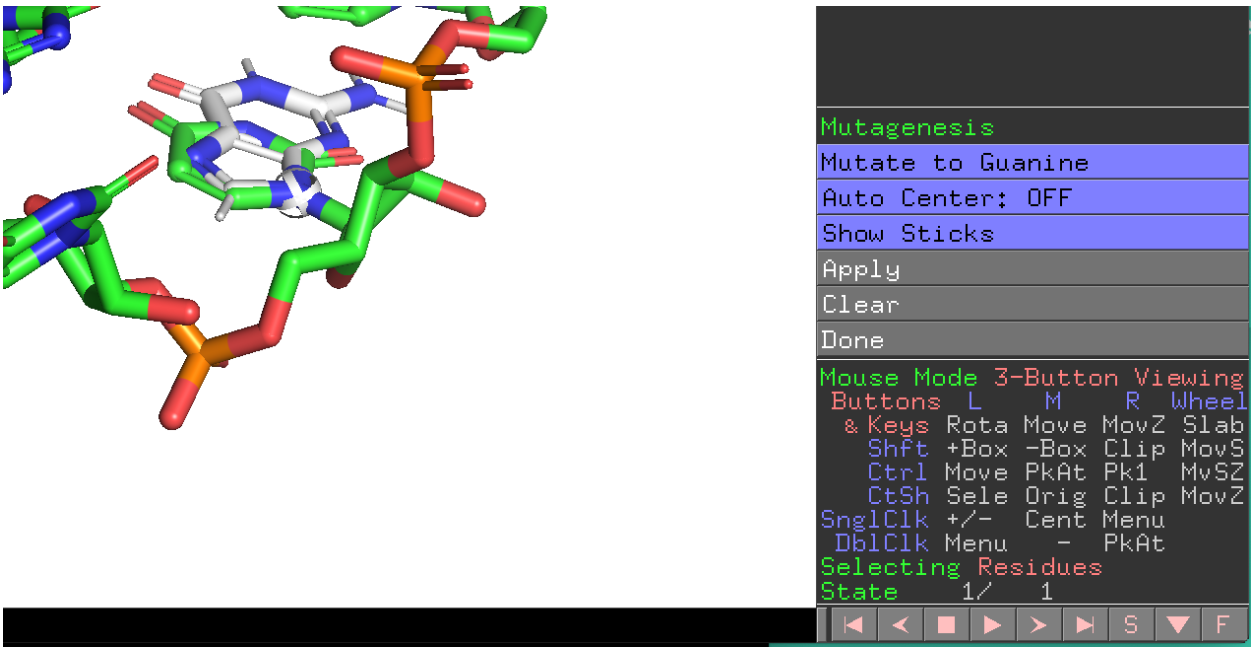
```
$ rna_pdb_tools.py --mutate 'A:1A+2A+3A+4A,B:13A' \
   --inplace output/205d_rmH2o_mutA1234-B1_inplace.pdb
```



Input structure on the left, mutated structure on the right.

If, for whatever reason, the tool here does not do what you want, use the tool from MC-Fold|MC-Sym Pipeline (go there https://www.major.iric.ca/MC-Pipeline/ and scroll down to the Section: "RNA SEQUENCE MUTATION" at the very bottom of the page).

Moreover, you can also mutate interactively proteins and nucleic acids with PyMOL >2.



Learn more here https://pymolwiki.org/index.php/Mutagenesis

If you want to mutate with PyMOL with command-line see this https://pymolwiki.org/index.php/Rotkit

2.11 add missing atoms

The tool is using the function:

`RNAStructure.`**`get_rnapuzzle_ready`**(*renumber_residues=True*, *fix_missing_atoms=True*, *rename_chains=True*, *ignore_op3=False*, *report_missing_atoms=True*, *keep_hetatm=False*, *backbone_only=False*, *no_backbone=False*, *bases_only=False*, *save_single_res=False*, *ref_frame_only=False*, *check_geometry=False*, *verbose=False*)

Get rnapuzzle (SimRNA) ready structure.

Clean up a structure, get current order of atoms.

Parameters

- **`renumber_residues`** – boolean, from 1 to ..., second chain starts from 1 etc.
- **`fix_missing_atoms`** – boolean, superimpose motifs from the minilibrary and copy-paste missing atoms, this is super crude, so should be used with caution.

Submission format @http://ahsoka.u-strasbg.fr/rnapuzzles/

Run `rna_tools.rna_tools.lib.RNAStructure.std_resn()` before this function to fix names.

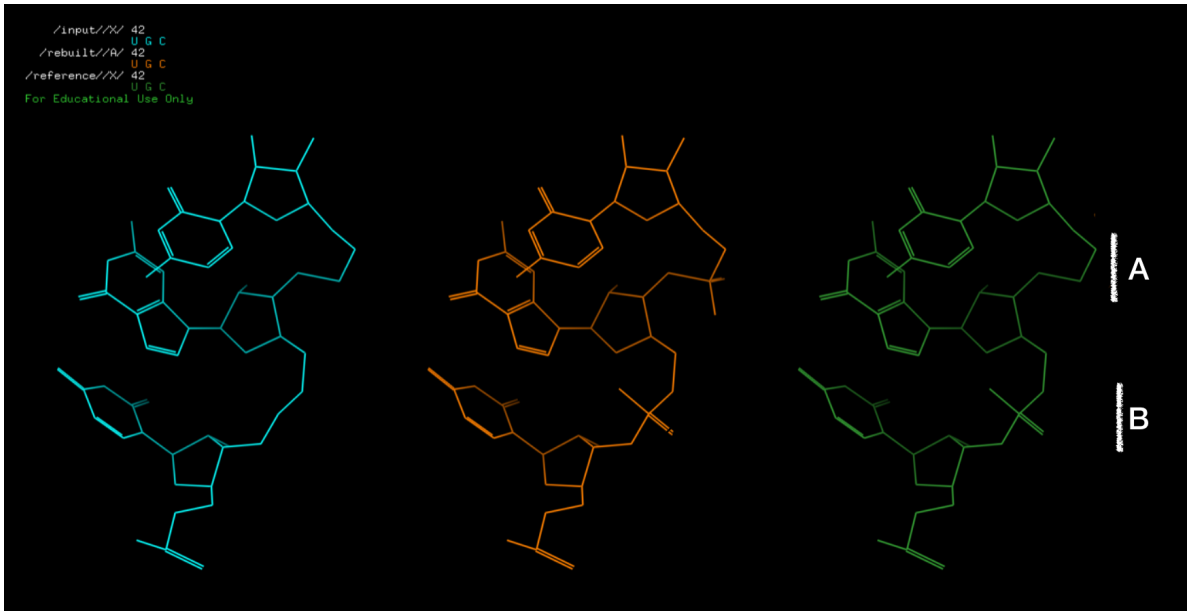


Figure: (Starting from left) input structure, structure with rebuilded atoms, and reference. The B fragment is observed in the reference used here as a "benchmark", fragment A is reconstructed atoms (not observed in the reference"). 201122

- 170305 Merged with get_simrna_ready and fixing OP3 terminal added
- 170308 Fix missing atoms for bases, and O2'

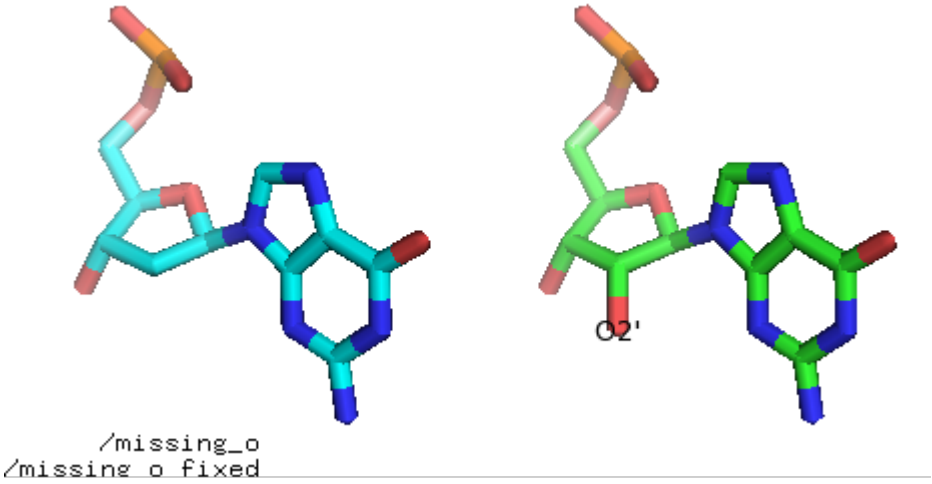


Fig. Add missing O2' atom (before and after).

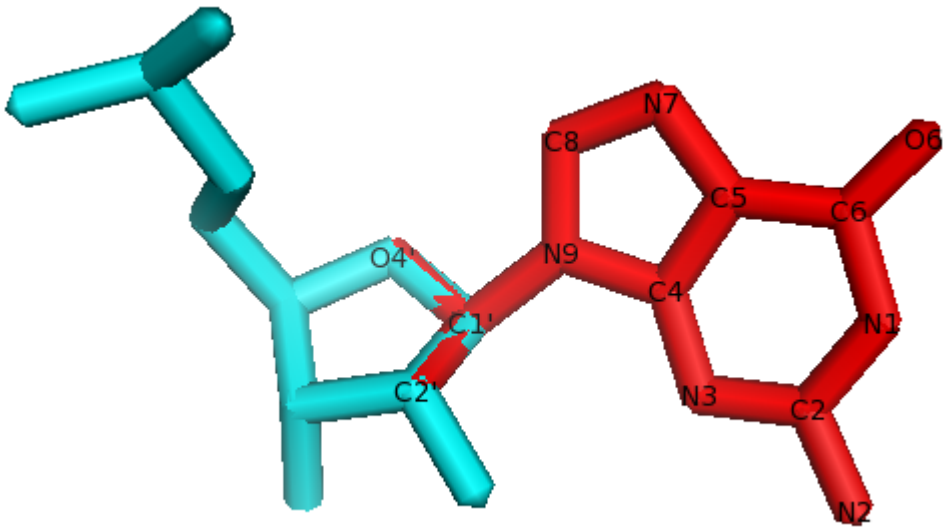


Fig. The residue to fix is in cyan. The G base from the library in red. Atoms O4', C2', C1' are shared between the sugar (in cyan) and the G base from the library (in red). These atoms are used to superimpose the G base on the sugar, and then all atoms from the base are copied to the residues.

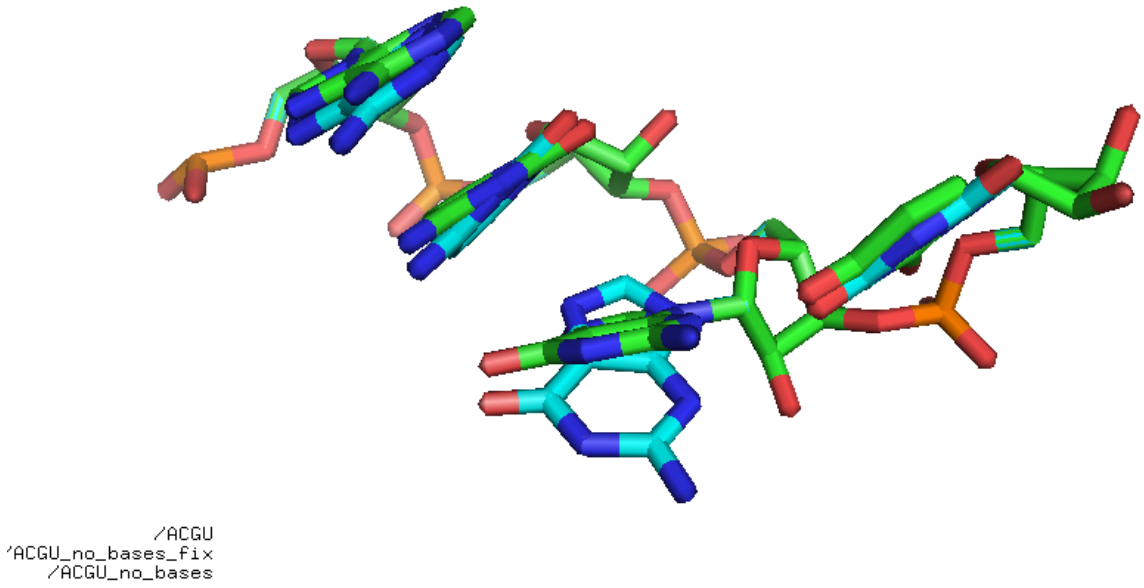


Fig. Rebuild ACGU base-less. It's not perfect but good enough for some applications.

Warning:	It was only tested with the whole base missing!

Warning:	requires: Biopython

Selection of atoms:

- posphate group (3x, OP1 ,P, OP2),
- connector (2x O5', C5'), /5x
- sugar (5x, C4', O4', C3', O3', C1', C2'), /10
- extra oxygens from sugar (2x, O2' O3'), for now it's /12!
- A (10x), G (11x), C (8x), U(8x), max 12+11=23

And 27 unique atoms: {'N9', 'O2', 'OP2', "O2'", "O4'", 'C8', "O3'", "C1'", 'C2', 'C6', "C5'", 'N6', 'C5', "C4'", 'C4', "O5'", "C3'", 'O6', 'N2', 'N7', 'OP1', 'N1', 'N4', 'P', "C2'", 'N3', 'O4'}.

CHAPTER

THREE

RNA-PDB-TOOLS

rna_pdb_tools - a swiss army knife to manipulation of RNA pdb structures

Remove atoms with XYZ equals 0:

```
(base)   MiniRoseTTA git:(main)  cat  4GXY_min_at0_chemicals.pdb
ATOM      1  OP1   G A   1      50.150  76.113  39.198  1.00  0.00
ATOM      2  P     G A   1      50.001  77.254  40.137  1.00  0.00
ATOM      3  OP2   G A   1      48.880  77.258  41.111  1.00  0.00
ATOM      4  O5'   G A   1      51.362  77.417  40.948  1.00  0.00
ATOM      5  C5'   G A   1       0.000   0.000   0.000  1.00  0.00
ATOM      6  C4'   G A   1       0.000   0.000   0.000  1.00  0.00
ATOM      7  O4'   G A   1       0.000   0.000   0.000  1.00  0.00
ATOM      8  C3'   G A   1       0.000   0.000   0.000  1.00  0.00
```

to get:

```
(base)   MiniRoseTTA git:(main)  rna_pdb_tools.py --remove0  4GXY_min_at0_chemicals.pdb
ATOM      1  OP1   G A   1      50.150  76.113  39.198  1.00  0.00
ATOM      2  P     G A   1      50.001  77.254  40.137  1.00  0.00
ATOM      3  OP2   G A   1      48.880  77.258  41.111  1.00  0.00
ATOM      4  O5'   G A   1      51.362  77.417  40.948  1.00  0.00
ATOM     35  OP1   C A   2      54.648  73.216  44.394  1.00  0.00
ATOM     36  P     C A   2      53.712  74.058  43.607  1.00  0.00
ATOM     37  OP2   C A   2      53.842  74.111  42.128  1.00  0.00
ATOM     38  O5'   C A   2      52.223  73.613  43.957  1.00  0.00
```

3.1 rna_pdb_tools

3.1.1 rna_pdb_tools.py

rna_pdb_tools - a swiss army knife to manipulation of RNA pdb structures

Usage:

```
$ rna_pdb_tools.py --delete A:46-56 --inplace *.pdb

 $ rna_pdb_tools.py --get-seq *
 # BujnickiLab_RNApuzzle14_n01bound
 > A:1-61
```

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```
# BujnickiLab_RNApuzzle14_n02bound
> A:1-61
CGUUAGCCCAGGAAACUGGGCGGAAGUAAGGCCCAUUGCACUCCGGGCCUGAAGCAACGCG
[...]
```

See *rna_pdb_merge_into_one.py* to merge PDB files in the order as you like into one NMR-like (multimodel) file

Examples:

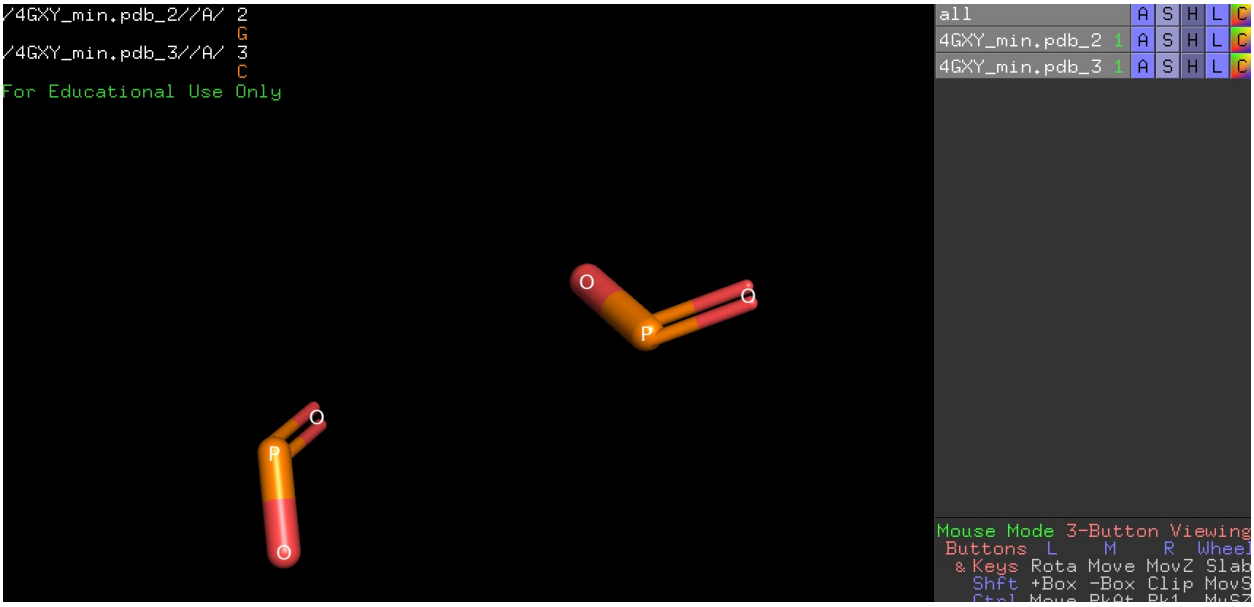
```
rna_pdb_tools.py --backbone-only   --get-rnapuzzle-ready  --inplace --suffix=bo examples/
↪4GXY_min.pdb
```

To extract specific atoms for each residue and write them to separate PDB file (next to the input files, following syntax "<input>_<resid>.pdb"):

```
rna_pdb_tools.py --rpr input/4GXY_min.pdb --save-single-res --ref-frame-only
```

Atoms presets:

```
--backbone-only       used only with --get-rnapuzzle-ready, keep only backbone (= remove␣
↪bases)
--ref-frame-only      used only with --get-rnapuzzle-ready, keep only reference frames,␣
↪OP1 OP2 P
--no-backbone         used only with --get-rnapuzzle-ready, remove atoms of backbone␣
↪(define as P OP1 OP2 O5')
--bases-only          used only with --get-rnapuzzle-ready, keep only atoms of bases
```



-v is for verbose, –version for version ;)

```
usage: rna_pdb_tools.py [-h] [--version] [-r] [--no-progress-bar]
                        [--renum-atoms] [--renum-nmr] [--renum-residues-dirty]
                        [--undo] [--delete-anisou] [--remove0] [--fix]
                        [--to-mol2] [--split-alt-locations] [-c] [--is-pdb]
                        [--is-nmr] [--nmr-dir NMR_DIR] [--un-nmr] [--orgmode]
```

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```
                        [--get-chain GET_CHAIN] [--fetch] [--fetch-ba]
                        [--fetch-chain] [--fetch-fasta] [--get-seq]
                        [--color-seq] [--ignore-files IGNORE_FILES]
                        [--compact] [--hide-warnings] [--get-ss]
                        [--rosetta2generic] [--no-hr] [--renumber-residues]
                        [--dont-rename-chains] [--dont-fix-missing-atoms]
                        [--inspect] [--collapsed-view] [--cv] [-v]
                        [--mutate MUTATE] [--edit EDIT]
                        [--rename-chain RENAME_CHAIN]
                        [--swap-chains SWAP_CHAINS] [--set-chain SET_CHAIN]
                        [--replace-chain REPLACE_CHAIN] [--delete DELETE]
                        [--extract EXTRACT] [--extract-chain EXTRACT_CHAIN]
                        [--uniq UNIQ] [--chain-first] [--oneline]
                        [--replace-htm] [--fasta] [--cif2pdb] [--pdb2cif]
                        [--mdr] [--get-rnapuzzle-ready] [--rpr]
                        [--keep-hetatm] [--inplace] [--here] [--suffix SUFFIX]
                        [--replace-hetatm] [--dont-report-missing-atoms]
                        [--backbone-only] [--ref-frame-only] [--no-backbone]
                        [--bases-only] [--save-single-res]
                        file [file ...]
```

file

file

-h, --help

show this help message and exit

--version

-r, --report

get report

--no-progress-bar

for –no-progress-bar for –rpr

--renum-atoms

renumber atoms, tested with –get-seq

--renum-nmr

--renum-residues-dirty

--undo

undo operation of action done –inplace, , rename “backup files” .pdb~ to pdb, ALL files in the folder, not only ~ related to the last action (that you might want to revert, so be careful)

--delete-anisou

remove files with ANISOU records, works with –inplace

--remove0

remove atoms of X=0 position

--fix

fix a PDB file, ! external program, pdbfixer used to fix missing atoms

--to-mol2

fix a PDB file, ! external program, pdbfixer used to fix missing atoms

--split-alt-locations

splits atoms, e.g. for alt locs A and B, it splits atoms two MODELS (all localizations A goes into MODEL1 and all localizations B goes into MODEL2

-c, --clean

get clean structure

--is-pdb

check if a file is in the pdb format

--is-nmr

check if a file is NMR-style multiple model pdb

--nmr-dir <nmr_dir>

make NMR-style multiple model pdb file from a set of files

rna_pdb_tools.py –nmr-dir . 'cwc15_u5_fragments*.pdb' > ~/Desktop/cwc15-u5.pdb

please use '' for pattern file recognition, this is a hack to deal with folders with thousands of models, if you used only *.pdb then the terminal will complain that you selected to many files.

--un-nmr

split NMR-style multiple model pdb files into individual models [biopython],

rna_pdb_tools.py –un-nmr split.pdb 2 /Users/magnus/Desktop/3hl2/split_1.pdb /Users/magnus/Desktop/3hl2/split_2.pdb

--orgmode

get a structure in org-mode format <sick!>

--get-chain <get_chain>

get chain, one or many, e.g, A, but now also ABC works

--fetch

fetch file from the PDB db, e.g., 1xjr, use 'rp' to fetch, fetch a given join, 4w90:C or 4w90_Cthe RNA-Puzzles standardized_dataset [around 100 MB]

--fetch-ba

fetch biological assembly from the PDB db

--fetch-chain

fetch a structure in extract chain, e.g. 6bk8 H

--fetch-fasta

fetch a fasta/sequence for given PDB ID, e.g. 6bk8

--get-seq

get seq

--color-seq

color seq, works with –get-seq

--ignore-files <ignore_files>

files to be ingored, .e.g, 'solution'

--compact

with –get-seq, get it in compact view' $ rna_pdb_tools.py –get-seq –compact *.pdb # 20_Bujnicki_1 ACCCGCAAGGCCGACGGCGCCGCCGCUGGUGCAAGUCCAGCCACGCUUCGGCGUGGGCGCUCAUGGGU # A:1-68 # 20_Bujnicki_2 ACCCGCAAGGCCGACGGCGCCGCCGCUGGUGCAAGUCCAGCCACGCUUCGGCGUGGGCGCUCAUGGGU # A:1-68 # 20_Bujnicki_3 ACCCGCAAGGCCGACGGCGCCGCCGCUGGUGCAAGUCCAGCCACGCUUCGGCGUGGGCGCUCAUGGGU # A:1-68 # 20_Bujnicki_4

--hide-warnings

hide warnings, works with –get-chain, it hides warnings that given changes are not detected in a PDB file

--get-ss

get secondary structure

--rosetta2generic

convert ROSETTA-like format to a generic pdb

--no-hr

do not insert the header into files

--renumber-residues

by defult is false

--dont-rename-chains

used only with –get-rnapuzzle-ready. By default: –get-rnapuzzle-ready rename chains from ABC.. to stop behavior switch on this option

--dont-fix-missing-atoms

used only with –get-rnapuzzle-ready

--inspect

inspect missing atoms (technically decorator to –get-rnapuzzle-ready without actually doing anything but giving a report on problems)

--collapsed-view

--cv

alias to collapsed_view

-v, --verbose

tell me more what you're doing, please!

--mutate <mutate>

mutate residues, e.g., –mutate "A:1a+2a+3a+4a,B:1a" to mutate to adenines the first four nucleotides of the chain A and the first nucleotide of the chain B

--edit <edit>

edit 'A:6>B:200', 'A:2-7>B:2-7'

--rename-chain <rename_chain>

edit 'A>B' to rename chain A to chain B

--swap-chains <swap_chains>

B>A, rename A to _, then B to A, then _ to B

--set-chain <set_chain>

set chain for all ATOM lines and TER (quite brutal function)

--replace-chain <replace_chain>

a file PDB name with one chain that will be used to replace the chain in the original PDB file, the chain id in this file has to be the same with the chain id of the original chain

--delete <delete>

delete the selected fragment, e.g. A:10-16, or for more than one fragment –delete 'A:1-25+30-57'

--extract <extract>

extract the selected fragment, e.g. A:10-16, or for more than one fragment –extract 'A:1-25+30-57', or even 'A:1-25+B:30-57'

--extract-chain <extract_chain>

extract chain, e.g. A

--uniq <uniq>

rna_pdb_tools.py –get-seq –uniq '[:5]' –compact –chain-first * | sort A:1-121 ACCUUGCGCAACUGGCGAAUCCUGGGGCUGCCGCCGGCAGUACCC...CA # rp13nc3295_min.out.1 A:1-123 ACCUUGCGCGACUGGCGAAUCCUGAAGCUGCUUUGAGCGGCUUCG...AG # rp13cp0016_min.out.1 A:1-123 ACCUUGCGCGACUGGCGAAUCCUGAAGCUGCUUUGAGCGGCUUCG...AG # zcp_6537608a_ALL-000001_AA A:1-45 57-71 GGGUCGUGACUGGCGAACAGGUGGGAAACCACCGGGGAGCGACCCGCCGCCCGCCUGGGC # solution

--chain-first

--oneline

--replace-htm

--fasta

with –get-seq, show sequences in fasta format, can be combined with –compact (mind, chains will be separated with ' ' in one line)

$ rna_pdb_tools.py –get-seq –fasta –compact input/20_Bujnicki_1.pdb > 20_Bujnicki_1 ACCCGCAAGGCCGACGGC GCCGCCGCUGGUGCAAGUCCAGCCACGCUUCGGCGUGGGCGCUCAUGGGU

--cif2pdb

[PyMOL Python package required]

--pdb2cif

[PyMOL Python package required]

--mdr

get structures ready for MD (like rpr but without first)

--get-rnapuzzle-ready

get RNApuzzle ready (keep only standard atoms).' Be default it does not renumber residues, use –renumber-residues [requires BioPython]

--rpr

alias to get_rnapuzzle ready)

--keep-hetatm

keep hetatoms

--inplace

in place edit the file! [experimental, only for get_rnapuzzle_ready, –delete, –get-ss, –get-seq, –edit-pdb]

--here

save a file next to the original file with auto suffix for –extract it's .extr.pdb

--suffix <suffix>

when used with –inplace allows you to change a name of a new file, –suffix del will give <file>_del.pdb (mind added _)

--replace-hetatm

replace 'HETATM' with 'ATOM' [tested only with –get-rnapuzzle-ready]

--dont-report-missing-atoms

used only with –get-rnapuzzle-ready

--backbone-only

used only with –get-rnapuzzle-ready, keep only backbone (= remove bases)

--ref-frame-only

used only with –get-rnapuzzle-ready, keep only reference frames, OP1 OP2 P

--no-backbone

used only with –get-rnapuzzle-ready, remove atoms of backbone (define as P OP1 OP2 O5')

--bases-only

used only with –get-rnapuzzle-ready, keep only atoms of bases

--save-single-res

used only with –get-rnapuzzle-ready, for each residue create a new pdb output file, you can combine it with –bases-only etc.

3.1.2 get RNAPuzzle ready

class rna_tools.rna_tools_lib.**RNAStructure**(*fn=''*)

RNAStructure - handles an RNA pdb file.

fn

path to the structural file, e.g., "../rna_tools/input/4ts2.pdb"

Type
string

name

filename of the structural file, "4ts2.pdb"

Type
string

lines

the PDB file is loaded and ATOM/HETATM/TER/END go to self.lines

Type
list

get_rnapuzzle_ready(*renumber_residues=True*, *fix_missing_atoms=True*, *rename_chains=True*, *ignore_op3=False*, *report_missing_atoms=True*, *keep_hetatm=False*, *backbone_only=False*, *no_backbone=False*, *bases_only=False*, *save_single_res=False*, *ref_frame_only=False*, *check_geometry=False*, *verbose=False*)

Get rnapuzzle (SimRNA) ready structure.

Clean up a structure, get current order of atoms.

Parameters

- **renumber_residues** – boolean, from 1 to ..., second chain starts from 1 etc.
- **fix_missing_atoms** – boolean, superimpose motifs from the minilibrary and copy-paste missing atoms, this is super crude, so should be used with caution.

Submission format @http://ahsoka.u-strasbg.fr/rnapuzzles/

Run `rna_tools.rna_tools.lib.RNAStructure.std_resn()` before this function to fix names.

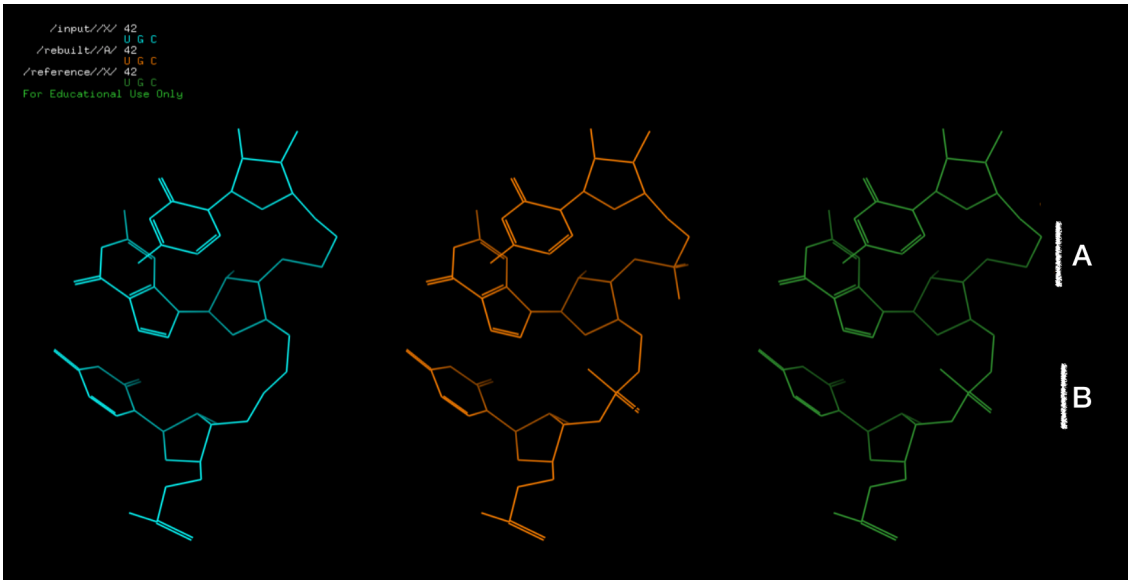


Figure: (Starting from left) input structure, structure with rebuilded atoms, and reference. The B fragment is observed in the reference used here as a "benchmark", fragment A is reconstructed atoms (not observed in the reference"). 201122

- 170305 Merged with get_simrna_ready and fixing OP3 terminal added
- 170308 Fix missing atoms for bases, and O2'

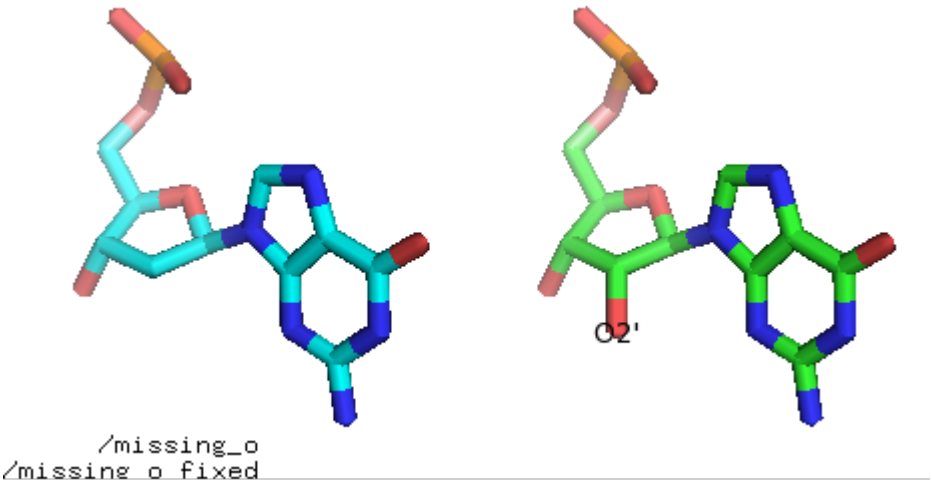


Fig. Add missing O2' atom (before and after).

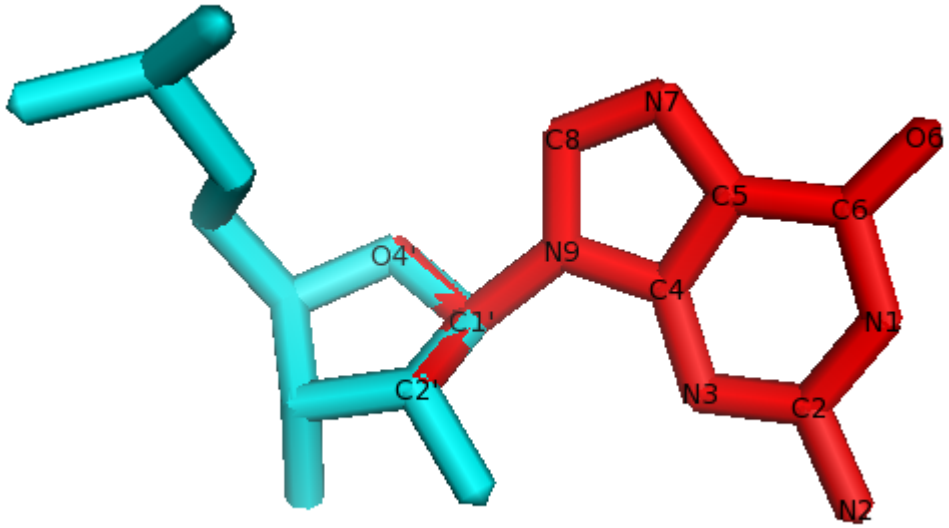


Fig. The residue to fix is in cyan. The G base from the library in red. Atoms O4', C2', C1' are shared between the sugar (in cyan) and the G base from the library (in red). These atoms are used to superimpose the G base on the sugar, and then all atoms from the base are copied to the residues.

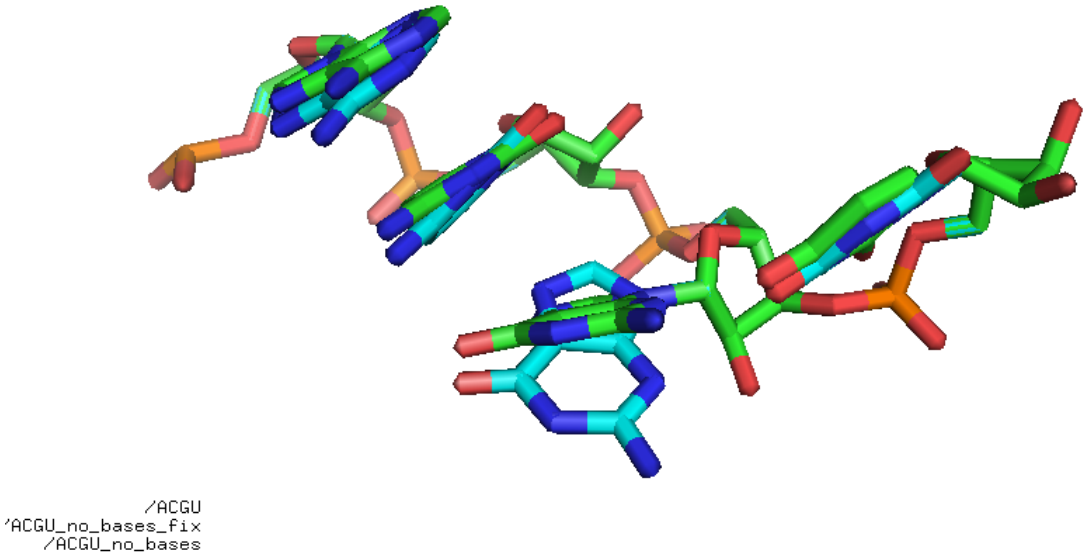


Fig. Rebuild ACGU base-less. It's not perfect but good enough for some applications.

Warning: It was only tested with the whole base missing!

Warning: requires: Biopython

Selection of atoms:

- posphate group (3x, OP1 ,P, OP2),
- connector (2x O5', C5'), /5x
- sugar (5x, C4', O4', C3', O3', C1', C2'), /10
- extra oxygens from sugar (2x, O2' O3'), for now it's /12!
- A (10x), G (11x), C (8x), U(8x), max 12+11=23

And 27 unique atoms: {'N9', 'O2', 'OP2', "O2'", "O4'", 'C8', "O3'", "C1'", 'C2', 'C6', "C5'", 'N6', 'C5', "C4'", 'C4', "O5'", "C3'", 'O6', 'N2', 'N7', 'OP1', 'N1', 'N4', 'P', "C2'", 'N3', 'O4'}.

3.1.3 get sequence

Example:

```
$ rna_pdb_tools.py --get-seq 5_solution_1.pdb
> 5_solution_1.pdb A:1-576
CAUCCGGUAUCCCAAGACAAUCUCGGGUUGGGUUGGGAAGUAUCAUGGCUAAUCACCAUGAUGCAAUCGGGUUGAACACUUAAUUGGGUUAAAACGGUGGGGGA
```

class rna_tools.rna_tools_lib.**RNAStructure**(*fn=''*)

RNAStructure - handles an RNA pdb file.

fn

path to the structural file, e.g., "../rna_tools/input/4ts2.pdb"

Type
string

name

filename of the structural file, "4ts2.pdb"

Type
string

lines

the PDB file is loaded and ATOM/HETATM/TER/END go to self.lines

Type
list

get_seq(*compact=False*, *chainfirst=False*, *fasta=False*, *addfn=''*, *color=False*)

Get seq (v2) gets segments of chains with correct numbering

Run:

```
python rna_pdb_seq.py input/1ykq_clx.pdb
> 1ykq_clx A:101-111
GGAGCUCGCCC
> 1ykq_clx B:201-238
GGGCGAGGCCGUGCCAGCUCUUCGGAGCAAUACUCGGC

> 6_solution_0 A:1-19 26-113 117-172
GGCGGCAGGUGCUCCCGACGUCGGGAGUUAAAAGGGAAG
```

Chains is {'A': {'header': 'A:1-19 26-113 117-172', 'resi': [1, 2, 3, ..., 19, 26, 27, ..., 172], 'seq': ['G', 'G', 'C', 'G', ... C', 'G', 'U', 'C']}}

Chains are in other as the appear in the file.

> **Warning:** take only ATOM and HETATM lines.

3.1.4 fetch

Example:

```
$ rna_pdb_tools.py --fetch 1xjr
downloading...1xjr ok
```

rna_tools.rna_tools_lib.**fetch**(*pdb_id*, *path='.'*)

fetch pdb file from RCSB.org https://files.rcsb.org/download/1Y26.pdb

Args: - pdb_id, but also a chain can be specified, 1jj2:A+B+C

Returns: - a path to a file

TODO: na_pdb_tools.py –extract A:1-25+B:30-57 1jj2.pdb

3.1.5 fetch Biological Assembly

Example:

```
$ rna_pdb_tools.py --fetch-ba 1xjr
downloading...1xjr_ba.pdb ok
```

or over a list of pdb ids in a text file:

```
$ cat data/pdb_ids.txt
1y26
1fir

$ while read p; do rna_pdb_tools.py --fetch-ba $p; done < data/pdb_ids.txt
downloading...1y26_ba.pdb ok
downloading...1fir_ba.pdb ok

$ ls *.pdb
1fir_ba.pdb 1y26_ba.pdb
```

rna_tools.rna_tools_lib.**fetch_ba**(*pdb_id*, *path='.'*)

fetch biological assembly pdb file from RCSB.org

```
>>> fetch_ba('1xjr')
...
```

3.1.6 delete

Examples:

```
$ for i in *pdb; do rna_pdb_tools.py --delete A:46-56 $i > ../rpr_rm_loop/$i ; done
```

go over all files in the current directory, remove a fragment of chain A, residues between 46-56 (including them) and save outputs to in the folder *rpr_rm_loops*.

3.1.7 edit

rna_tools.rna_tools_lib.**edit_pdb**(*f*, *args*)

Edit your structure.

The function can take `A:3-21>A:1-19` or even syntax like this `A:3-21>A:1-19,B:22-32>B:20-30` and will do an editing.

The output is printed, line by line. Only ATOM lines are edited!

Examples:

```
$ rna_pdb_tools.py --edit 'A:3-21>A:1-19' 1f27_clean.pdb > 1f27_clean_A1-19.pdb
```

or even:

```
$ rna_pdb_tools.py --edit 'A:3-21>A:1-19,B:22-32>B:20-30' 1f27_clean.pdb > 1f27_
↪clean_renumb.pdb
```

3.1.8 RNAStructure (rna_tools_lib)

rna_tools_lib.py - main lib file, many tools in this lib is using this file.

exception rna_tools.rna_tools_lib.**MethodUnknown**

exception rna_tools.rna_tools_lib.**PDBFetchError**

class rna_tools.rna_tools_lib.**RNAStructure**(*fn=''*)

RNAStructure - handles an RNA pdb file.

fn

path to the structural file, e.g., "../rna_tools/input/4ts2.pdb"

Type
string

name

filename of the structural file, "4ts2.pdb"

Type
string

lines

the PDB file is loaded and ATOM/HETATM/TER/END go to self.lines

Type
list

check_geometry(*verbose=False*)

Check for correct "Polymer linkage, it should be around 1.6Å with a sigma around 0.01.

Carrascoza, F., Antczak, M., Miao, Z., Westhof, E. & Szachniuk, M. Evaluation of the stereochemical quality of predicted RNA 3D models in the RNA-Puzzles submissions. Rna 28, 250–262 (2022).

Values for 1xjr.pdb:

```
op.mean(): 1.599316
op.std(): 0.009274074

po.mean(): 1.5984017
po.std(): 0.0069191623
```

requires biopython

edit_occupancy_of_pdb(*pdb*, *pdb_out*, *v=False*)

Make all atoms 1 (flexi) and then set occupancy 0 for seletected atoms. Return False if error. True if OK

fix_O_in_UC()

fix_op_atoms()

Replace OXP' to OPX1, e.g ('O1P' -> 'OP1')

fix_with_qrnas(*outfn=''*, *verbose=False*)

Add missing heavy atom.

A residue is recognized base on a residue names.

Copy QRNAS folder to curr folder, run QRNAS and remove QRNAS.

> **Warning:** QRNAS required (http://genesilico.pl/QRNAS/QRNAS.tgz)

get_all_chain_ids()

Returns
chain ids, e.g. set(['A', 'B'])
Return type
set

get_atom_code(*line*)

Get atom code from a line of a PDB file

get_atom_coords(*line*)

Get atom coordinates from a line of a PDB file

get_atom_num(*line*)

Extract atom number from a line of PDB file :param * line = ATOM line from a PDB file:
Output:

- atom number (int)

get_info_chains()

return A:3-21 B:22-32

get_remarks_text()

Get remarks as text for given file. This function re-open files, as define as self.fn to get remarks.

Example:

```
r = RNAStructure(fout)
remarks = r.get_remarks_txt()
r1 = r.get_res_txt('A', 1)
r2 = r.get_res_txt('A', 2)
r3 = r.get_res_txt('A', 3)
with open(fout, 'w') as f:
    f.write(remarks)
    f.write(r1)
    f.write(r2)
    f.write(r3)

remarks is

REMARK 250 Model edited with rna-tools
REMARK 250  ver 3.5.4+63.g4338516.dirty
REMARK 250  https://github.com/mmagnus/rna-tools
REMARK 250  Fri Nov 13 10:15:19 2020
```

get_report()

Returns
report, messages collected on the way of parsing this file

Return type
string

get_res_code(*line*)

Get residue code from a line of a PDB file

get_res_num(*line*)

Extract residue number from a line of PDB file :param * line = ATOM line from a PDB file:
Output:

- residue number as an integer

get_res_text(*chain_id*, *resi*)

Get a residue of given resi of chain_id and return as a text

Parameters

- **chain_id** (*str*) – e.g., 'A'
- **resi** (*int*) – e.g., 1

Return type
txt

Example:

```
r = RNAStructure(fn)
print(r.get_res_txt('A', 1))

ATOM      1  O5'   G A   1      78.080 -14.909  -0.104  1.00  9.24      ␣
↪     O
ATOM      2  C5'   G A   1      79.070 -15.499  -0.956  1.00  9.70      ␣
↪     C
ATOM      3  C4'   G A   1      78.597 -16.765  -1.648  1.00  9.64      ␣
```

(continues on next page)

(continued from previous page)

```
↪      C
ATOM      4  O4'   G A   1      78.180 -17.761  -0.672  1.00  9.88      ␣
↪      O
(...)
```

get_rnapuzzle_ready(*renumber_residues=True*, *fix_missing_atoms=True*, *rename_chains=True*, *ignore_op3=False*, *report_missing_atoms=True*, *keep_hetatm=False*, *backbone_only=False*, *no_backbone=False*, *bases_only=False*, *save_single_res=False*, *ref_frame_only=False*, *check_geometry=False*, *verbose=False*)

Get rnapuzzle (SimRNA) ready structure.

Clean up a structure, get current order of atoms.

Parameters

- **renumber_residues** – boolean, from 1 to …, second chain starts from 1 etc.
- **fix_missing_atoms** – boolean, superimpose motifs from the minilibrary and copy-paste missing atoms, this is super crude, so should be used with caution.

Submission format @http://ahsoka.u-strasbg.fr/rnapuzzles/

Run `rna_tools.rna_tools.lib.RNAStructure.std_resn()` before this function to fix names.

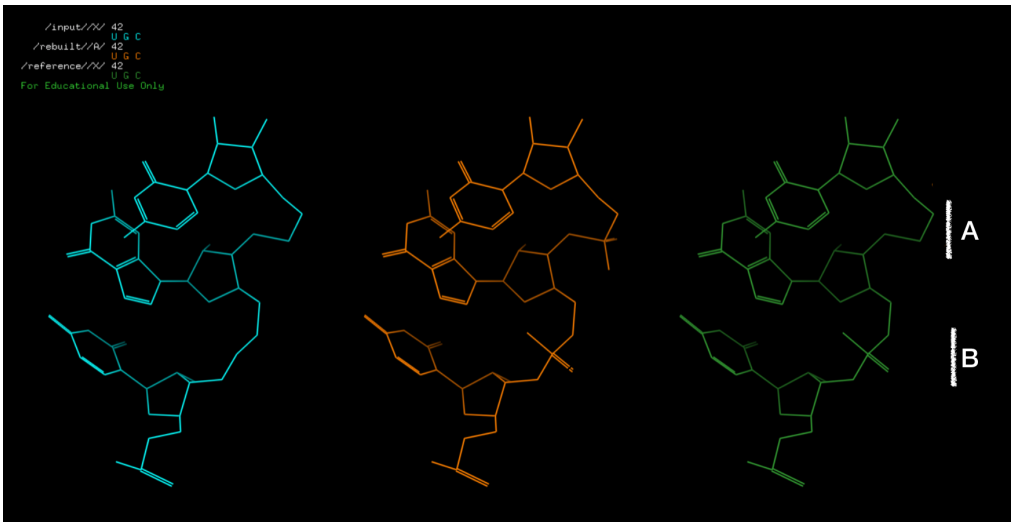


Figure: (Starting from left) input structure, structure with rebuilded atoms, and reference. The B fragment is observed in the reference used here as a "benchmark", fragment A is reconstructed atoms (not observed in the reference"). 201122

- 170305 Merged with get_simrna_ready and fixing OP3 terminal added
- 170308 Fix missing atoms for bases, and O2'

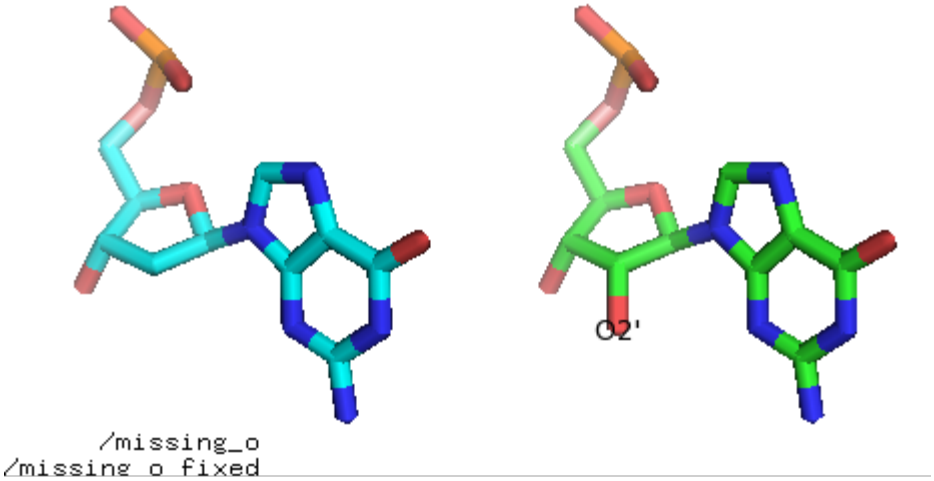


Fig. Add missing O2' atom (before and after).

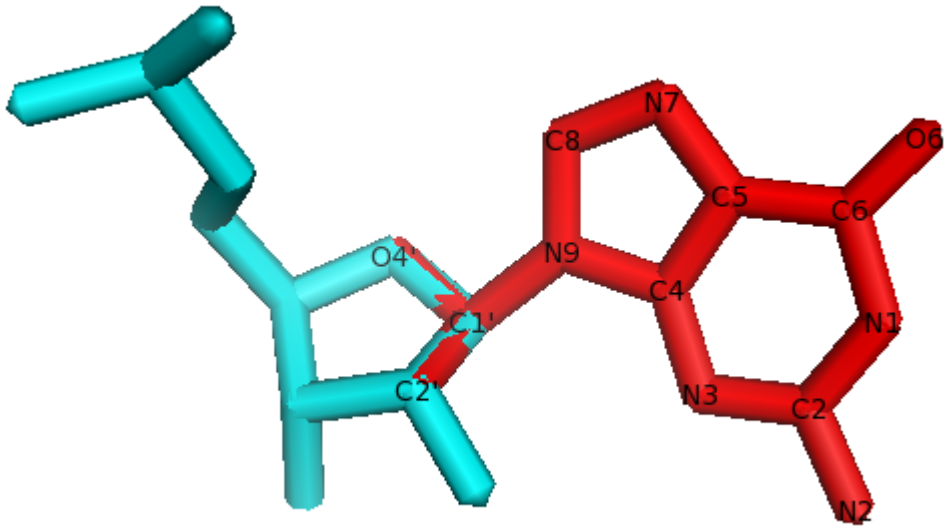


Fig. The residue to fix is in cyan. The G base from the library in red. Atoms O4', C2', C1' are shared between the sugar (in cyan) and the G base from the library (in red). These atoms are used to superimpose the G base on the sugar, and then all atoms from the base are copied to the residues.

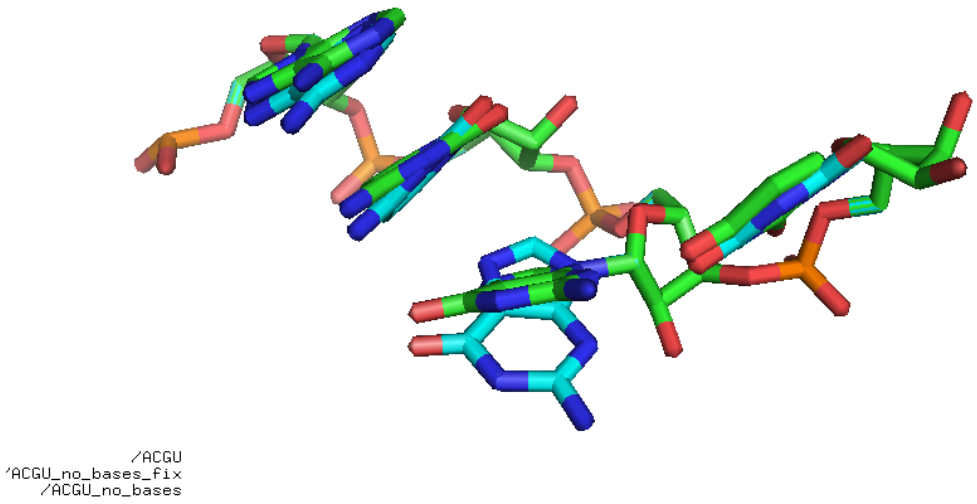


Fig. Rebuild ACGU base-less. It's not perfect but good enough for some applications.

> **Warning:** It was only tested with the whole base missing!

> **Warning:** requires: Biopython

Selection of atoms:

- posphate group (3x, OP1 ,P, OP2),
- connector (2x O5', C5'), /5x
- sugar (5x, C4', O4', C3', O3', C1', C2'), /10
- extra oxygens from sugar (2x, O2' O3'), for now it's /12!
- A (10x), G (11x), C (8x), U(8x), max 12+11=23

And 27 unique atoms: {'N9', 'O2', 'OP2', "O2'", "O4'", 'C8', "O3'", "C1'", 'C2', 'C6', "C5'", 'N6', 'C5', "C4'", 'C4', "O5'", "C3'", 'O6', 'N2', 'N7', 'OP1', 'N1', 'N4', 'P', "C2'", 'N3', 'O4'}.

`get_seq`(*compact=False*, *chainfirst=False*, *fasta=False*, *addfn=''*, *color=False*)

Get seq (v2) gets segments of chains with correct numbering

Run:

```
python rna_pdb_seq.py input/1ykq_clx.pdb
> 1ykq_clx A:101-111
GGAGCUCGCCC
> 1ykq_clx B:201-238
GGGCGAGGCCGUGCCAGCUCUUCGGAGCAAUACUCGGC

> 6_solution_0 A:1-19 26-113 117-172
GGCGGCAGGUGCUCCCGACGUCGGGAGUUAAAAGGGAAG
```

Chains is `{'A': {'header': 'A:1-19 26-113 117-172', 'resi': [1, 2, 3, ..., 19, 26, 27, ..., 172], 'seq': ['G', 'G', 'C', 'G', ... C', 'G', 'U', 'C']}}`

Chains are in other as the appear in the file.

> **Warning:** take only ATOM and HETATM lines.

get_text(*add_end=True*)

works on self.lines.

is_amber_like()

Use self.lines and check if there is XX line

is_mol2()

Return True if is_mol2 based on the presence of `@<TRIPOS>`.

is_nmr()

True if the file is an NMR-style multiple model pdb

Returns
True or Fo

Return type
boolean

is_pdb()

Return True if the files is in PDB format.

If self.lines is empty it means that nothing was parsed into the PDB format.

reload()

Reload the object.

remove(*verbose*)

Delete file, self.fn

remove_ion()

TER 1025 U A 47 HETATM 1026 MG MG A 101 42.664 34.395 50.249 1.00 70.99 MG HETATM 1027 MG MG A 201 47.865 33.919 48.090 1.00 67.09 MG

rtype
object

remove_water()

Remove HOH and TIP3

rename_chain(*chain_id_old*, *chain_id_new*, *debug=False*)

Rename chains

Parameters
- **chain_id_old** (*str*) – e.g., A
- **chain_id_new** (*str*) – e.g., B
- **debug** (*bool*) – show some diagnostics

Returns
pdb content (txt) self.lines is updated with new lines

renum_atoms()

Renum atoms, from 1 to X for line; ATOM/HETATM

set_atom_code(*line*, *code*)

Add atom name/code:
ATOM 1 OP2 C A 1 29.615 36.892 42.657 1.00 1.00 O
^^^ ^ and element

set_atom_coords(*line*, *x*, *y*, *z*)

Get atom coordinates from a line of a PDB file

set_atom_occupancy(*line*, *occupancy*)

set occupancy for line

set_occupancy_atoms(*occupancy*)

Parameters
occupancy –

set_res_code(*line*, *code*)

Parameters
- **lines** –
- **code** –

path (str): The path of the file to wrap field_storage (FileStorage): The :class:Y instance to wrap temporary (bool): Whether or not to delete the file when the File instance is destructed

Returns
A buffered writable file descriptor

Return type
BufferedFileStorage

std_resn()

'Fix' residue names which means to change them to standard, e.g. RA5 -> A

Works on self.lines, and returns the result to self.lines.

Will change things like:

```
# URI -> U, URA -> U
1xjr_clx_charmm.pdb:ATOM    101  P   URA A   5      58.180  39.153  30.
↪336  1.00 70.94
rp13_Dokholyan_1_URI_CYT_ADE_GUA_hydrogens.pdb:ATOM  82  P   URI A   4 ␣
↪   501.633 506.561 506.256  1.00  0.00          P
```

un_nmr(*startwith1=True*, *directory=''*, *verbose=False*)

Un NMR - Split NMR-style multiple model pdb files into individual models.
Take self.fn and create new files in the way:

```
input/1a9l_NMR_1_2_models.pdb
   input/1a9l_NMR_1_2_models_0.pdb
   input/1a9l_NMR_1_2_models_1.pdb
```

Warning: This function requires biopython.

rna_pdb_tools.py –un-nmr AF-Q5TCX8-F1-model_v1_core_Ctrim_mdr_MD.pdb

36

cat *MD_* > md.pdb

write(*outfn=''*, *verbose=False*)

Write `self.lines` to a file (and add END file)

Parameters
- **outfn** (*str*) – file to save, if outfn is '', then simply use self.fn
- **verbose** (*Boolen*) – be verbose or not

Returns
None

rna_tools.rna_tools_lib.**aa3to1**(*aaa*)

based on https://pymolwiki.org/index.php/Aa_codes

rna_tools.rna_tools_lib.**collapsed_view**(*args*)

Collapsed view of pdb file. Only lines with C5' atoms are shown and TER, MODEL, END.

example:

```
[mm] rna_tools git:(master) $ python rna-pdb-tools.py --cv input/1f27.pdb
ATOM      1  C5'   A A   3      25.674  19.091   3.459  1.00 16.99           C
ATOM     23  C5'   C A   4      19.700  19.206   5.034  1.00 12.65           C
ATOM     43  C5'   C A   5      14.537  16.130   6.444  1.00  8.74           C
ATOM     63  C5'   G A   6      11.726  11.579   9.544  1.00  9.81           C
ATOM     86  C5'   U A   7      12.007   7.281  13.726  1.00 11.35           C
ATOM    106  C5'   C A   8      12.087   6.601  18.999  1.00 12.74           C
TER
```

rna_tools.rna_tools_lib.**edit_pdb**(*f*, *args*)

Edit your structure.

The function can take `A:3-21>A:1-19` or even syntax like this `A:3-21>A:1-19,B:22-32>B:20-30` and will do an editing.

The output is printed, line by line. Only ATOM lines are edited!

Examples:

```
$ rna_pdb_tools.py --edit 'A:3-21>A:1-19' 1f27_clean.pdb > 1f27_clean_A1-19.pdb
```

or even:

```
$ rna_pdb_tools.py --edit 'A:3-21>A:1-19,B:22-32>B:20-30' 1f27_clean.pdb > 1f27_clean_renumb.pdb
```

rna_tools.rna_tools_lib.**fetch**(*pdb_id*, *path='.'*)

fetch pdb file from RCSB.org https://files.rcsb.org/download/1Y26.pdb

Args: - pdb_id, but also a chain can be specified, 1jj2:A+B+C

Returns: - a path to a file

TODO: na_pdb_tools.py –extract A:1-25+B:30-57 1jj2.pdb

rna_tools.rna_tools_lib.**fetch_ba**(*pdb_id*, *path='.'*)

fetch biological assembly pdb file from RCSB.org

```
>>> fetch_ba('1xjr')
...
```

rna_tools.rna_tools_lib.**fetch_cif_ba**(*cif_id*, *path='.'*)

fetch biological assembly cif file from RCSB.org

rna_tools.rna_tools_lib.**get_rna_tools_path**()

Return path to the rt.

rna_tools.rna_tools_lib.**load_rnas**(*path*, *verbose=True*)

Load structural files (via glob) and return a list of RNAStructure objects.

Examples:

```
rnas = rtl.load_rnas('../rna_tools/input/mq/*.pdb')
```

rna_tools.rna_tools_lib.**replace_atoms**(*struc_fn*, *insert_fn*, *verbose=False*)

Replace XYZ coordinate of the file (struc_fn) with XYZ from another file (insert_fn).

This can be useful if you want to replace positions of atoms, for example, one base only. The lines are muted based on atom name, residue name, chain, residue index (marked with XXXX below).:

ATOM 11 N1 A 2 27 303.441 273.472 301.457 1.00 0.00 N # file ATOM 1 N1 A 2 27 300.402 273.627 303.188 1.00 99.99 N # insert ATOM 11 N1 A 2 27 300.402 273.627 303.188 1.00 0.00 N # inserted

XXXXXXXXXXXXXXXX # part used to find lines to be replaced

ATOM 1 P A 2 27 295.653 270.783 300.135 1.00119.29 P # next line

Parameters

- **struc_fn** (*str*) – path to the main PDB file
- **insert_fn** (*str*) – path to the file that will be injected in into the main PDB file

Returns
text in the PDB format

Return type
string

rna_tools.rna_tools_lib.**replace_chain**(*struc_fn*, *insert_fn*, *chain_id*)

Replace chain of the main file (struc_fn) with some new chain (insert_fn) of given chain id.

Parameters

- **struc_fn** (*str*) – path to the main PDB file
- **insert_fn** (*str*) – path to the file that will be injected in into the main PDB file
- **chain_id** (*str*) – chain that will be inserted into the main PDB file

Returns
text in the PDB format

Return type
string

rna_tools.rna_tools_lib.**set_chain_for_struc**(*struc_fn*, *chain_id*, *save_file_inplace=False*, *skip_ter=True*)

Quick & dirty function to set open a fn PDB format, set chain_id and save it to a file. Takes only lines with ATOM and TER.

rna_tools.rna_tools_lib.**sort_strings**(*l*)

Sort the given list in the way that humans expect. http://blog.codinghorror.com/sorting-for-humans-natural-sort-order/

3.2 Standardize your PDB files

3.2.1 rna_standardize.py

rna_standardize.py - standardzie RNA PDB structures

Usage:

```
$ rna_standardize.py <pdb file>
```

-v is for verbose, –version for version ;)

```
usage: rna_standardize.py [-h] [--version] [--no-progress-bar] [--renum-nmr]
                          [--inplace] [-v] [--dont-replace-hetatm]
                          [--keep-hetatm] [--here] [--no-hr]
                          [--check-geometry] [--dont-fix-missing-atoms]
                          [--mdr] [--renumber-residues] [--suffix SUFFIX]
                          [--dont-report-missing-atoms] [--dont-rename-chains]
                          [--backbone-only] [--no-backbone] [--bases-only]
                          file [file ...]
```

file

file

-h, --help

show this help message and exit

--version

--no-progress-bar

for –no-progress-bar for –rpr

--renum-nmr

--inplace

in place edit the file! [experimental, only for get_rnapuzzle_ready, –delete, –get-ss, –get-seq, –edit-pdb]

-v, --verbose

tell me more what you're doing, please!

--dont-replace-hetatm

replace 'HETATM' with 'ATOM' [tested only with –get-rnapuzzle-ready]

--keep-hetatm

keep hetatoms, [if not replaced anyway with ATOM, see –dont-replace-hetatm

--here

save a file next to the original file with auto suffix for –extract it's .extr.pdb

--no-hr

do not insert the header into files

--check-geometry

check connectivity betweeen residues and angles

--dont-fix-missing-atoms

used only with –get-rnapuzzle-ready

--mdr

get structures ready for MD (like rpr but without first)

--renumber-residues

by defult is false

--suffix <suffix>

when used with –inplace allows you to change a name of a new file, –suffix del will give <file>_del.pdb (mind added _)

--dont-report-missing-atoms

used only with –get-rnapuzzle-ready

--dont-rename-chains

used only with –get-rnapuzzle-ready. By default: –get-rnapuzzle-ready rename chains from ABC.. to stop behavior switch on this option

--backbone-only

used only with –get-rnapuzzle-ready, keep only backbone (= remove bases)

--no-backbone

used only with –get-rnapuzzle-ready, remove atoms of backbone (define as P OP1 OP2 O5')

--bases-only

used only with –get-rnapuzzle-ready, keep only atoms of bases

class rna_tools.rna_tools_lib.**RNAStructure**(*fn=''*)

RNAStructure - handles an RNA pdb file.

fn

path to the structural file, e.g., "../rna_tools/input/4ts2.pdb"

Type
string

name

filename of the structural file, "4ts2.pdb"

Type
string

lines

the PDB file is loaded and ATOM/HETATM/TER/END go to self.lines

Type
list

get_rnapuzzle_ready(*renumber_residues=True*, *fix_missing_atoms=True*, *rename_chains=True*, *ignore_op3=False*, *report_missing_atoms=True*, *keep_hetatm=False*, *backbone_only=False*, *no_backbone=False*, *bases_only=False*, *save_single_res=False*, *ref_frame_only=False*, *check_geometry=False*, *verbose=False*)

Get rnapuzzle (SimRNA) ready structure.

Clean up a structure, get current order of atoms.

Parameters

- **renumber_residues** – boolean, from 1 to ..., second chain starts from 1 etc.
- **fix_missing_atoms** – boolean, superimpose motifs from the minilibrary and copy-paste missing atoms, this is super crude, so should be used with caution.

Submission format @http://ahsoka.u-strasbg.fr/rnapuzzles/

Run `rna_tools.rna_tools.lib.RNAStructure.std_resn()` before this function to fix names.

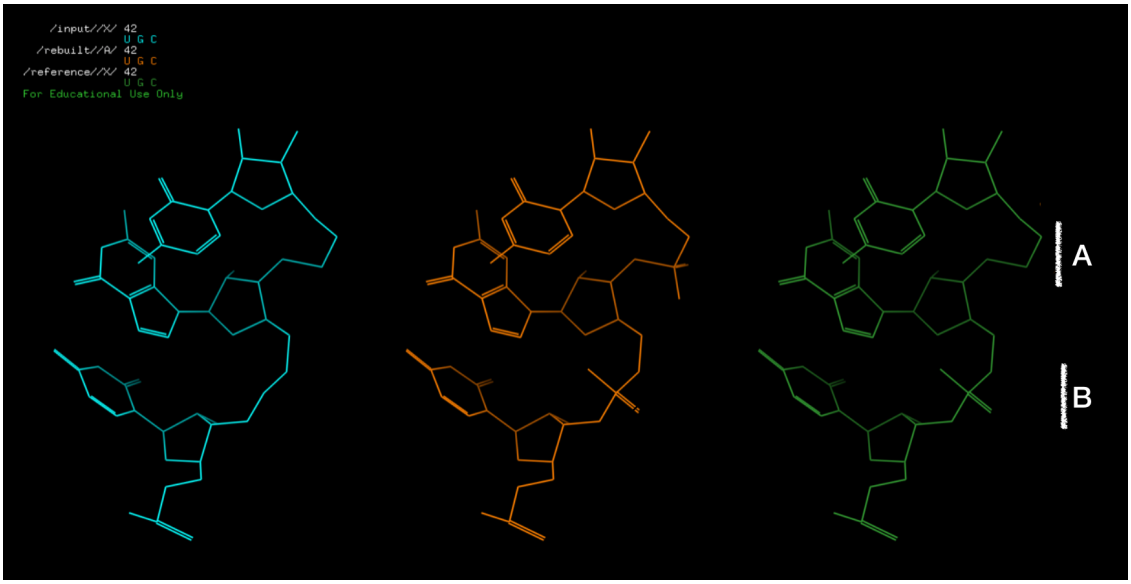


Figure: (Starting from left) input structure, structure with rebuilded atoms, and reference. The B fragment is observed in the reference used here as a "benchmark", fragment A is reconstructed atoms (not observed in the reference"). 201122

- 170305 Merged with get_simrna_ready and fixing OP3 terminal added
- 170308 Fix missing atoms for bases, and O2'

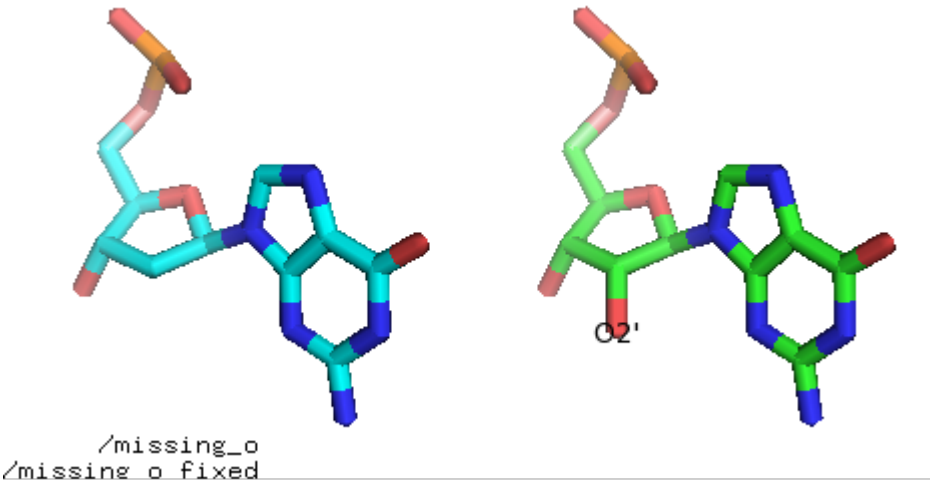


Fig. Add missing O2' atom (before and after).

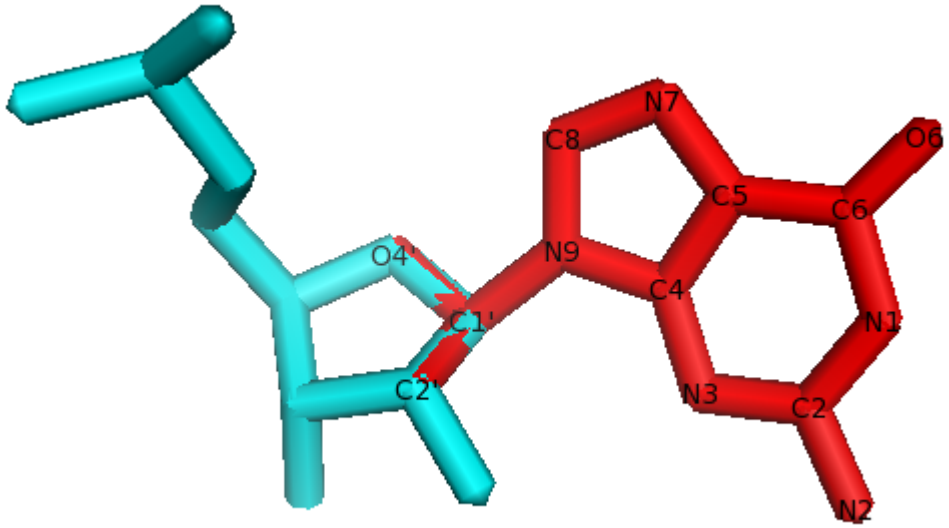


Fig. The residue to fix is in cyan. The G base from the library in red. Atoms O4', C2', C1' are shared between the sugar (in cyan) and the G base from the library (in red). These atoms are used to superimpose the G base on the sugar, and then all atoms from the base are copied to the residues.

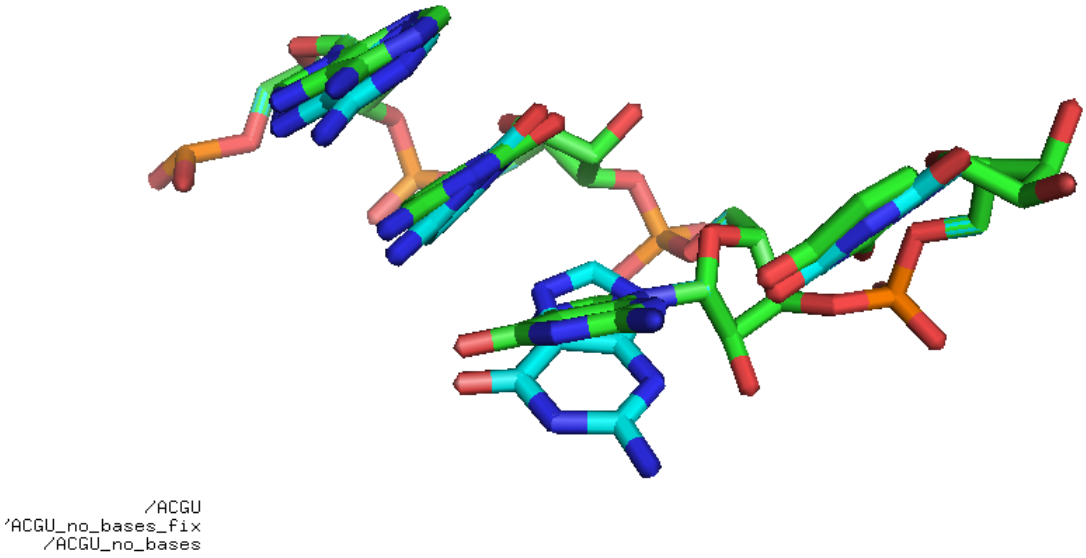


Fig. Rebuild ACGU base-less. It's not perfect but good enough for some applications.

Warning: It was only tested with the whole base missing!

Warning: requires: Biopython

Selection of atoms:

- posphate group (3x, OP1 ,P, OP2),
- connector (2x O5', C5'), /5x
- sugar (5x, C4', O4', C3', O3', C1', C2'), /10
- extra oxygens from sugar (2x, O2' O3'), for now it's /12!
- A (10x), G (11x), C (8x), U(8x), max 12+11=23

And 27 unique atoms: {'N9', 'O2', 'OP2', "O2'", "O4'", 'C8', "O3'", "C1'", 'C2', 'C6', "C5'", 'N6', 'C5', "C4'", 'C4', "O5'", "C3'", 'O6', 'N2', 'N7', 'OP1', 'N1', 'N4', 'P', "C2'", 'N3', 'O4'}.

3.2.2 Atoms order

Atoms order, A as an example:

```
ATOM      1  P     G A   1      50.626  49.730  50.573  1.00100.19           P
ATOM      2  OP1   G A   1      49.854  48.893  49.562  1.00100.19           O
ATOM      3  OP2   G A   1      52.137  49.542  50.511  1.00 99.21           O
ATOM      4  O5'   G A   1      50.161  49.136  52.023  1.00 99.82           O
ATOM      5  C5'   G A   1      50.216  49.948  53.210  1.00 98.63           C
ATOM      6  C4'   G A   1      50.968  49.231  54.309  1.00 97.84           C
ATOM      7  O4'   G A   1      50.450  47.888  54.472  1.00 97.10           O
ATOM      8  C3'   G A   1      52.454  49.030  54.074  1.00 98.07           C
ATOM      9  O3'   G A   1      53.203  50.177  54.425  1.00 99.39           O
ATOM     10  C2'   G A   1      52.781  47.831  54.957  1.00 96.96           C
ATOM     11  O2'   G A   1      53.018  48.156  56.313  1.00 96.77           O
ATOM     12  C1'   G A   1      51.502  47.007  54.836  1.00 95.70           C
ATOM     13  N9    G A   1      51.628  45.992  53.798  1.00 93.67           N
ATOM     14  C8    G A   1      51.064  46.007  52.547  1.00 92.60           C
ATOM     15  N7    G A   1      51.379  44.966  51.831  1.00 91.19           N
ATOM     16  C5    G A   1      52.197  44.218  52.658  1.00 91.47           C
ATOM     17  C6    G A   1      52.848  42.992  52.425  1.00 90.68           C
ATOM     18  O6    G A   1      52.826  42.291  51.404  1.00 90.38           O
ATOM     19  N1    G A   1      53.588  42.588  53.534  1.00 90.71           N
ATOM     20  C2    G A   1      53.685  43.282  54.716  1.00 91.21           C
ATOM     21  N2    G A   1      54.452  42.733  55.671  1.00 91.23           N
ATOM     22  N3    G A   1      53.077  44.429  54.946  1.00 91.92           N
ATOM     23  C4    G A   1      52.356  44.836  53.879  1.00 92.62           C

ATOM     24  P     C A   2      54.635  50.420  53.741  1.00100.19           P
ATOM     25  OP1   C A   2      55.145  51.726  54.238  1.00100.19           O
```

3.2.3 OP3

The first residue will have only OP1 and OP2 (OP3 will be removed):

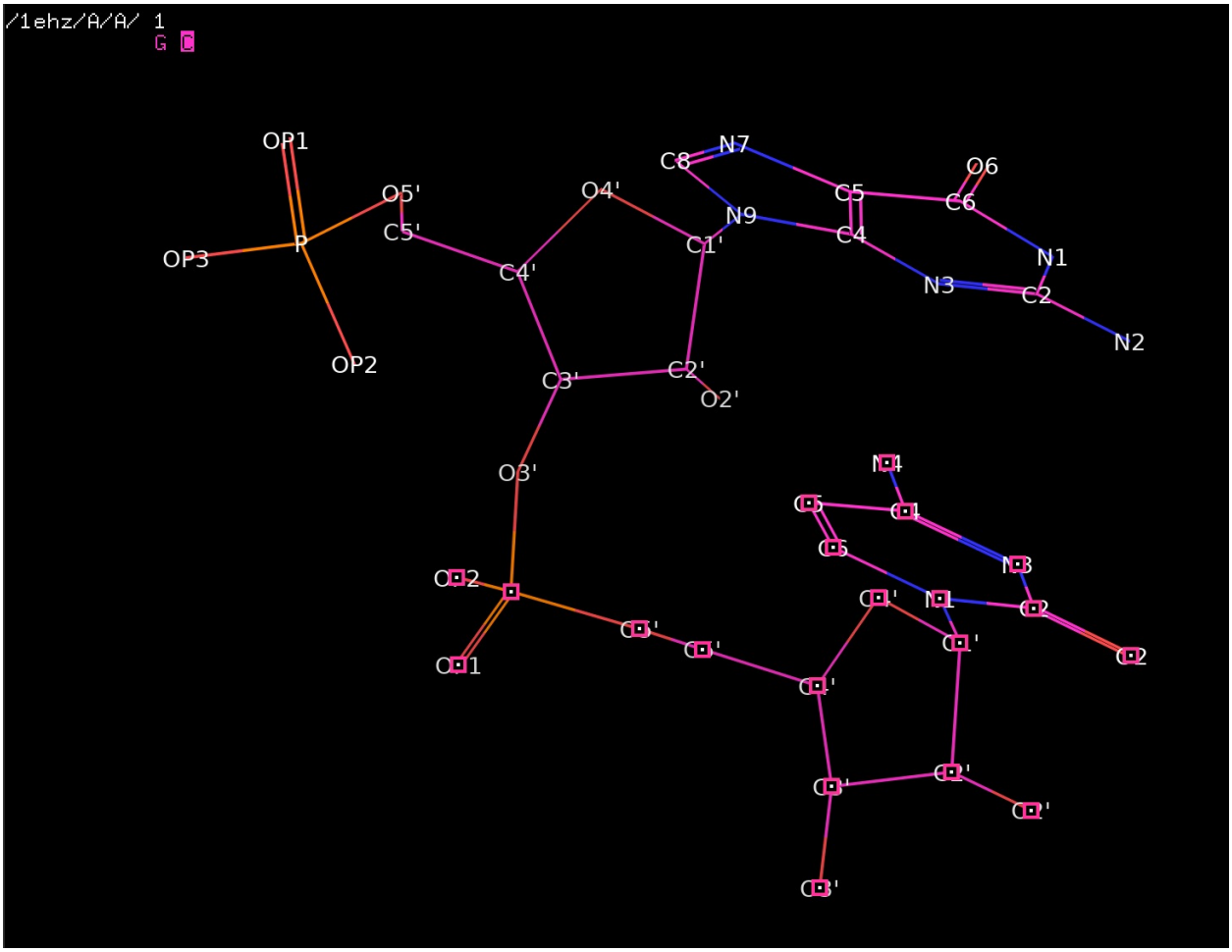
```
ATOM      1  OP3   G A   1      50.193  51.190  50.534  1.00 99.85           O
ATOM      2  P     G A   1      50.626  49.730  50.573  1.00100.19           P
ATOM      3  OP1   G A   1      49.854  48.893  49.562  1.00100.19           O
ATOM      4  OP2   G A   1      52.137  49.542  50.511  1.00 99.21           O
ATOM      5  O5'   G A   1      50.161  49.136  52.023  1.00 99.82           O
```

(continues on next page)

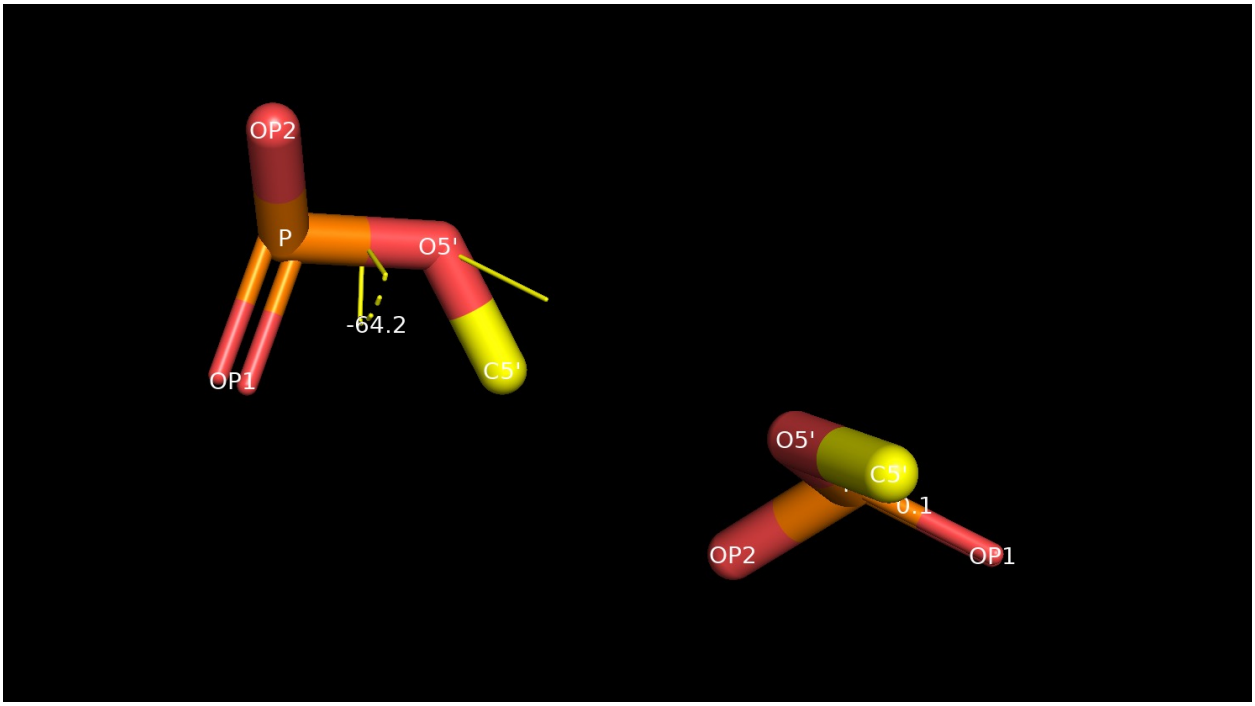
(continued from previous page)

```
ATOM      6  C5'   G A   1      50.216  49.948  53.210  1.00 98.63           C
ATOM      7  C4'   G A   1      50.968  49.231  54.309  1.00 97.84           C
```

Listing. An example: *1ehz.pdb*.



3.3 Torsion angle analysis



3.3.1 rna_torsions.py

Examples:

```
$ rna_torsions.py ./input/4GXY_min.pdb
f, alphaprime, beta
input ./input/4GXY_min.pdb <Residue G het=  resseq=2 icode= >, -64.20924484900823, -143.
↪18546007904766
input ./input/4GXY_min.pdb <Residue C het=  resseq=3 icode= >, 2.3394112025736815, 70.
↪4052871669199
```

Comparison:

```
$ rna_x3dna.py input/4GXY_min.pdb -s
input: input/4GXY_min.pdb
   nt id   res  alpha   beta  gamma  delta  epsilon  zeta      e-z           chi     ␣
↪phase-angle sugar-type  ssZp    Dp  splay     paired
0   1  G  A.G2    NaN -143.2  153.7   82.5    -92.3 -31.9  -60(..)  -179.0(anti)  19.5(C3
↪'-endo)  ~C3'-endo  4.39  4.56  18.32  no paired
1   2  C  A.C3 -111.4   70.4  160.0   80.6      NaN   NaN      NaN  -177.6(anti)  11.1(C3
↪'-endo)  ~C3'-endo   NaN   NaN    NaN  no paired
```

```
usage: rna_torsions.py [-h] [-v] file
```

file

-h, --help
show this help message and exit

-v, --verbose
be verbose

3.4 PDB Edit Bfactor/Occupancy

3.4.1 rna_pdb_edit_occupancy_bfactor.py

rna_pdb_edit_occupancy_bfactor.py - edit occupancy or bfactor in PDB file.

Example:

```
rna_pdb_edit_occupancy_bfactor.py --occupancy --select A:1-40,B:1-22 \
                                  --set-to 0 \
                                  19_Bujnicki_Human_4_rpr_n0-000001.pdb


rna_pdb_edit_occupancy_bfactor.py --occupancy \
                                   --select A:1-2 \
                                   --select-atoms P+C4\' \
                                   --set-to 10 \
                                   -o test_data/3w3s_homologymodel_out.PD
                                   --set-not-selected-to 8
                                   test_data/3w3s_homologymodel.pdb
```

```
usage: rna_pdb_edit_occupancy_bfactor.py [-h] (--bfactor | --occupancy)
                                         [--select SELECT] [--set-to SET_TO]
                                         [--set-not-selected-to SET_NOT_SELECTED_TO]
                                         [-o OUTPUT] [--verbose]
                                         [--select-atoms SELECT_ATOMS]
                                         file
```

file
file

-h, --help
show this help message and exit

--bfactor
set bfactor

--occupancy
set occupancy

--select <select>
get chain, e.g A:1-10, works also for multiple chainse.g A:1-40,B:1-22

--set-to <set_to>
set value to, default is 1

--set-not-selected-to <set_not_selected_to>
set value to, default is 0

-o <output>, **--output** <output>

file output

--verbose

be verbose

--select-atoms <select_atoms>

select only given atomscan be only one atom, e.g. Por more, use ' for prims, e.g. P+C4'

rna_tools.tools.rna_pdb_edit_occupancy_bfactor.rna_pdb_edit_occupancy_bfactor.**edit_occupancy_of_pdb**(*txt*, *pdb*, *pdb_* *bfac* *tor*, *oc-* *cu-* *pan* *set_* *set_* *se-* *lect_* *v=F*

Change ouccupancy or bfactor of pdb file.

Load the structure, and first set everything to be *set_not_selected_to* and then set selected to *sel_to*.

Parameters

- **txt** (*str*) – A:1-10, selection, what to change
- **pdb** (*str*) – filename to read as an input
- **pdb_out** (*str*) – filename to save an output
- **bfactor** (*bool*) – if edit bfactor
- **occupancy** (*bool*) – if edit occupancy
- **set_to** (*float*) – set to this value, if within selection
- **set_not_selected_to** (*float*) – set to this value, if not within selection
- **select_atoms** (*str*) – P, P+C4', use + as a separator
- **v** (*bool*) – be verbose

Returns

if OK, save an output to pdb_out

Return type

bool

Warning: this function requires BioPython

3.5 Add chain to a file

Example:

```
./rna_add_chain.py -c X ../../input/1msy_rnakbmd_decoy999_clx_noChain.pdb     > ../../
↪output/1msy_rnakbmd_decoy999_clx_noChain_Xchain.pdb
```

From:

```
ATOM      1  O5'   U     1      42.778  25.208  46.287  1.00  0.00
ATOM      2  C5'   U     1      42.780  26.630  45.876  1.00  0.00
ATOM      3  C4'   U     1      42.080  27.526  46.956  1.00  0.00
ATOM      4  O4'   U     1      43.013  28.044  47.963  1.00  0.00
ATOM      5  C1'   U     1      42.706  29.395  48.257  1.00  0.00
ATOM      6  N1    U     1      43.857  30.305  47.703  1.00  0.00
ATOM      7  C6    U     1      45.057  29.857  47.308  1.00  0.00
ATOM      8  C5    U     1      46.025  30.676  46.763  1.00  0.00
ATOM      9  C4    U     1      45.720  32.110  46.702  1.00  0.00
ATOM     10  O4    U     1      46.444  32.975  46.256  1.00  0.00
```

to:

```
ATOM      1  O5'   U X   1      42.778  25.208  46.287  1.00  0.00
ATOM      2  C5'   U X   1      42.780  26.630  45.876  1.00  0.00
ATOM      3  C4'   U X   1      42.080  27.526  46.956  1.00  0.00
ATOM      4  O4'   U X   1      43.013  28.044  47.963  1.00  0.00
ATOM      5  C1'   U X   1      42.706  29.395  48.257  1.00  0.00
ATOM      6  N1    U X   1      43.857  30.305  47.703  1.00  0.00
ATOM      7  C6    U X   1      45.057  29.857  47.308  1.00  0.00
ATOM      8  C5    U X   1      46.025  30.676  46.763  1.00  0.00
ATOM      9  C4    U X   1      45.720  32.110  46.702  1.00  0.00
ATOM     10  O4    U X   1      46.444  32.975  46.256  1.00  0.00
```

in a loop:

```
for i in *; do rna_add_chain.py -c A $i > ../struc/${i}; done
```

rna_tools.tools.misc.rna_add_chain.**get_parser**()

3.5.1 rna_add_chain.py

```
usage: rna_add_chain.py [-h] [-c CHAIN] file
```

file
file

-h, **--help**
show this help message and exit

-c <chain>, **--chain** <chain>
a new chain, e.g. A

3.6 Measure distance between atoms

3.6.1 pdbs_measure_atom_dists.py

This is a quick and dirty method of comparison two RNA structures (stored in pdb files). It measures the distance between the relevan atoms (C4') for nucleotides defined as "x" in the sequence alignment.

author: F. Stefaniak, modified by A. Zyla, supervision of mmagnus

```
usage: pdbs_measure_atom_dists.py [-h] [-v]
                                  seqid1 seqid2 alignfn pdbfn1 pdbfn2
```

seqid1

seq1 id in the alignemnt

seqid2

seq2 id in the alignemnt

alignfn

alignemnt in the Fasta format

pdbfn1

pdb file1

pdbfn2

pdb file2

-h, --help

show this help message and exit

-v, --verbose

increase output verbosity

This is a quick and dirty method of comparison two RNA structures (stored in pdb files). It measures the distance between the relevan atoms (C4') for nucleotides defined as "x" in the sequence alignment.

author: F. Stefaniak, modified by A. Zyla, supervision of mmagnus

rna_tools.tools.pdbs_measure_atom_dists.pdbs_measure_atom_dists.**find_core**(*seq_with_gaps1*, *seq_with_gaps2*)

.

Parameters

- **seq_with_gaps1** (*str*) – a sequence 1 from the alignment
- **seq_with_gaps1** – a sequence 2 from the alignment

Usage:

```
>>> find_core('GUUCAG------------------UGAC-', 'CUUCGCAGCCAUUGCACUCCGGCUGCGAUG')
'xxxxxx------------------xxxx-'
```

Returns

core="xxxxxx————————-xxxx-"

rna_tools.tools.pdbs_measure_atom_dists.pdbs_measure_atom_dists.**get_parser**()

rna_tools.tools.pdbs_measure_atom_dists.pdbs_measure_atom_dists.**get_seq**(*alignfn*, *seqid*)

Get seq from an alignment with gaps.

Parameters

- **alignfn** (*str*) – a path to an alignment
- **seqid** (*str*) – seq id in an alignment

Usage:

```
>>> get_seq('test_data/ALN_OBJ1_OBJ2.fa', 'obj1')
SeqRecord(seq=SeqRecord(seq=Seq('GUUCAG------------------UGAC-',␣
↪SingleLetterAlphabet()), id='obj1', name='obj1', description='obj1', dbxrefs=[]),␣
↪id='<unknown id>', name='<unknown name>', description='<unknown description>',␣
↪dbxrefs=[])
```

Returns

SeqRecord

rna_tools.tools.pdbs_measure_atom_dists.pdbs_measure_atom_dists.**map_coords_atom**(*structure*)

.

Args: structure (pdb): PDB Biopython object: with a pdb structure

Returns

a list of coords for atoms structure1realNumber: a list of residues

Return type

struct1dict

rna_tools.tools.pdbs_measure_atom_dists.pdbs_measure_atom_dists.**open_pdb**(*pdbfn*)

Open pdb with Biopython.

Parameters

pdbfn1 (*str*) – a path to a pdb structure

Returns

with a pdb structure

Return type

PDB Biopython object

CHAPTER

FOUR

RNA-TOOLS

4.1 RNA Sequence

RNA Sequence with secondary structure prediction methods.

This tool takes a given sequence and returns the secondary structure prediction provided by 5 different tools: RNAfold, RNAsubopt, ipknot, contextfold and centroid_fold. You must have these tools installed. You don't have to install all tools if you want to use only one of the methods.

It's easy to add more methods of your choince to this class.

4.1.1 Installation

Depends on what tools you want to use, follow the instructions below.

4.1.1.1 ContextFold

https://www.cs.bgu.ac.il/~negevcb/contextfold/

needs Java. Try this on Ubuntu 14-04 https://askubuntu.com/questions/521145/how-to-install-oracle-java-on-ubuntu-14-04 Single chain only!

4.1.1.2 ViennaRNA

https://www.tbi.univie.ac.at/RNA/

For OSX install from the binary Installer from the page.

4.1.1.3 ipknot OSX

https://github.com/satoken/homebrew-rnatools

If one encounters a problem:

```
[mm] Desktop$ /usr/local/opt/bin/ipknot
dyld: Library not loaded: /usr/local/opt/glpk/lib/libglpk.40.dylib
  Referenced from: /usr/local/opt/bin/ipknot
  Reason: image not found
[1]    51654 abort      /usr/local/opt/bin/ipknot
```

the solution is:

```
brew install glpk # on OSX
```

4.1.1.4 RNA Structure

http://rna.urmc.rochester.edu/

Works with 5.8.1; Jun 16, 2016.

Download http://rna.urmc.rochester.edu/RNAstructureDownload.html and untar it in <RNA_PDB_TOOLS>/opt/RNAstructure/; run make, the tools will be compiled in a folder exe. Set up DATPATH in your bashrc to <RNA_PDB_TOOLS>/opt/RNAstructure/data_tables DATAPATH=/home/magnus/work/src/rna-pdb-tools/opt/RNAstructure/data_tables/ (read more http://rna.urmc.rochester.edu/Text/Thermodynamics.html). RNAstructure can be run with SHAPE restraints, read more http://rna.urmc.rochester.edu/Text/File_Formats.html#Constraint about the format. The file format for SHAPE reactivity comprises two columns. The first column is the nucleotide number, and the second is the reactivity. Nucleotides for which there is no SHAPE data can either be left out of the file, or the reactivity can be entered as less than -500. Columns are separated by any white space.

4.1.1.5 MC-Sym

4.1.2 FAQ

- Does it work for more than one chain??? Hmm.. I think it's not. You have to check on your own. –magnus

4.1.3 TIPS

Should you need to run it on a list of sequences, use the following script:

```
from rna_tools import Seq
f = open("listOfSequences.fasta")
for line in f:
 if line.startswith('>'):
   print line,
 else:
   print line,
   s = Seq.Seq(line.strip()) # module first Seq and class second Seq #without strip this␣
↪has two lines
   print s.predict_ss(method="contextfold"),
   #print s.predict_ss(method="centroid_fold")
```

Todo:

- This calss should be renamed to RNASeq and merged with RNASeq class from RNAalignment

exception rna_tools.Seq.**MethodNotChosen**

class rna_tools.Seq.**RNASequence**(*seq*, *ss=''*, *name='rna_seq'*)

RNASequence.

Usage:

```
>>> seq = RNASequence("CCCCUUUUGGGG")
>>> seq.name = 'RNA03'
>>> print(seq.predict_ss("RNAfold", constraints="((((....))))"))
>RNA03
CCCCUUUUGGGG
((((....)))) ( -6.40)
```

eval(*ss=''*, *no_dangling_end_energies=False*, *verbose=False*)

Evaluate energy of RNA sequence.

Parameters

- **ss** (*optional*) –
- **no_dangling_end_energies** (*Boolean*) –
- **verbose** (*Boolean*) –

Returns

Energy (float)

The RNAeval web server calculates the energy of a RNA sequence on a given secondary structure. You can use it to get a detailed thermodynamic description (loop free-energy decomposition) of your RNA structures.

Simply paste or upload your sequence below and click Proceed. To get more information on the meaning of the options click the help symbols. You can test the server using this sample sequence/structure pair.

An equivalent RNAeval command line call would have been:

```
RNAeval -v -d0 < input.txt
```

Read more: <http://rna.tbi.univie.ac.at//cgi-bin/RNAWebSuite/RNAeval.cgi>

get_foldability(*ss=''*, *verbose=False*)

Calculate foldability based on EntRNA.

Steps:

- parse SS into basepairs,
- calculate foldabilty

Configuration:

- Set ENTRNA_PATH to the folder where ENTRNA_predict.py is.

Cmd wrapper in here:

```
python ENTRNA_predict.py --seq_file pseudoknotted_seq.txt --str_file␣
↪pseudoknotted_str.txt
```

Su, C., Weir, J. D., Zhang, F., Yan, H., & Wu, T. (2019). ENTRNA: a framework to predict RNA foldability. BMC Bioinformatics, 20(1), 1–11. http://doi.org/10.1186/s12859-019-2948-5

predict_ss(*method='RNAfold'*, *constraints=''*, *enforce_constraint=False*, *shapefn=''*, *explore=''*, *verbose=0*, *path=''*)

Predict secondary structure of the seq.

Parameters

- **method** – {mcfold, RNAfold}

- **onstraints** –
- **shapefn** (*str*) – path to a file with shape reactivites
- **verbose** (*boolean*) –

It creates a seq fasta file and runs various methods for secondary structure prediction. You can provide also a constraints file for RNAfold and RNAsubopt.

Methods that can be used with contraints: RNAsubopt, RNAfold, mcfold.

Methods that can be used with SHAPE contraints: RNAfold.

ContextFold

Example:

```
$ java -cp bin contextFold.app.Predict in:CCCCUUUGGGGG
CCCCUUUGGGGG
((((....))))
```

It seems that a seq has to be longer than 9. Otherwise:

```
$ java -cp bin contextFold.app.Predict in:UUUUUUGGG
Exception in thread "main" java.lang.ArrayIndexOutOfBoundsException: 10

# this is OK
$ java -cp bin contextFold.app.Predict in:CCCCUUUGGG
CCCCUUUGGG
.(((...)))
```

RNAstructure

Example:

```
>>> seq = RNASequence("GGGGUUUUCCC")
>>> print(seq.predict_ss("rnastructure"))
>  ENERGY = -4.4  rna_seq
GGGGUUUUCCC
((((...))))
```

and with the shape data:

```
>>> print(seq.predict_ss("rnastructure", shapefn="data/shape.txt"))
>  ENERGY = -0.2  rna_seq
GGGGUUUUCCC
.(((....)))
```

the shape data:

```
1 10
2 1
3 1
```

You can easily see that the first G is unpaired right now! The reactivity of this G was set to 10. Worked!

MC-Fold

MC-Fold uses the online version of the tool, this is very powerful with constraints:

```
rna_seq
acucggcuaggcgaguauaaaauagccgucaggccuagcgcguccaagccuagccccuucuggggcugggcgaagggucggg
((((........))))........((((..............((((((((((((((....))))))))))))))..
↪))))
curl -Y 0 -y 300 -F "pass=lucy" -F mask="((((........))))........((((............
↪..((((((((((((((....))))))))))))))..))))" -F sequence=
↪"acucggcuaggcgaguauaaaauagccgucaggccuagcgcguccaagccuagccccuucuggggcugggcgaagggucggg
↪" https://www.major.iric.ca/cgi-bin/MC-Fold/mcfold.static.cgi
mcfold::energy best dynamics programming: -53.91
(-53.91, '((((........))))........((((..............((((((((((((((....
↪))))))))))))))..))))')

curl -Y 0 -y 300 -F "pass=lucy" -F mask="((((........))))........((((............
↪..((((((((((..............))))))))))..))))" -F sequence=
↪"acucggcuaggcgaguauaaaauagccgucaggccuagcgcguccaagccuagccccuucuggggcugggcgaagggucggg
↪" https://www.major.iric.ca/cgi-bin/MC-Fold/mcfold.static.cgi
mcfold::energy best dynamics programming: -34.77
(-34.77, '((((........))))........((((..............((((((((((.............
↪))))))))))..))))')

acucggcuaggcgaguauaaaauagccgucaggccuagcgcguccaagccuagccccuucuggggcugggcgaagggucggg
((((........))))........((((..............((((((((((((((....))))))))))))))..
↪))))
curl -Y 0 -y 300 -F "pass=lucy" -F mask=
↪"((((xxxxxxxx))))xxxxxxx((((xxxxxxxxxxxxxx((((((((((xxxxxxxxxxxxxx))))))))))xx))))
↪" -F sequence=
↪"acucggcuaggcgaguauaaaauagccgucaggccuagcgcguccaagccuagccccuucuggggcugggcgaagggucggg
↪" https://www.major.iric.ca/cgi-bin/MC-Fold/mcfold.static.cgi
mcfold::energy best dynamics programming: -34.77
(-34.77, '((((........))))........((((..............((((((((((.............
↪))))))))))..))))')


acucggcuaggcgaguauaaaauagccgucaggccuagcgcguccaagccuagccccuucuggggcugggcgaagggucggg
((((........))))........((((..............((((((((((((((....))))))))))))))..
↪))))
curl -Y 0 -y 300 -F "pass=lucy" -F mask=
↪"((((********))))*******((((**************(((((((((**************)))))))))**))))
↪" -F sequence=
↪"acucggcuaggcgaguauaaaauagccgucaggccuagcgcguccaagccuagccccuucuggggcugggcgaagggucggg
↪" https://www.major.iric.ca/cgi-bin/MC-Fold/mcfold.static.cgi
mcfold::energy best dynamics programming: -77.30
(-71.12, '(((((((..)))))))........((((((.(((...))))..((((((((((((((....
↪))))))))))))))))))')

acucggcuaggcgaguauaaaauagccgucaggccuagcgcguccaagccuagccccuucuggggcugggcgaagggucggg
((((........))))........((((..............((((((((((((((....))))))))))))))..
↪))))
curl -Y 0 -y 300 -F "pass=lucy" -F mask=
↪"((((**[[[[[**))))*******((((****]]]]]****((((((((((((((((****))))))))))))))))**))))
↪" -F sequence=
↪"acucggcuaggcgaguauaaaauagccgucaggccuagcgcguccaagccuagccccuucuggggcugggcgaagggucggg
↪" https://www.major.iric.ca/cgi-bin/MC-Fold/mcfold.static.cgi
```

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```
mcfold::energy best dynamics programming: -77.30
('-77.30',
 ↪'((((**[[[[[**))))*******((((****]]]]]****(((((((((((((((****)))))))))))))))**))))
 ↪')
```

explore

The sub-optimal search space can be constrained within a percentage of the minimum free energy structure, as MC-fold makes use of the Waterman-Byers algorithm [18, 19]. Because the exploration has an exponential time complexity, increasing this value can have a dramatic effect on MC-Fold's run time.

Parisien, M., & Major, F. (2009). RNA Modeling Using the MC-Fold and MC-Sym Pipeline [Manual] (pp. 1–84).

rna_tools.Seq.**load_fasta_ss_into_RNAseqs**(*fn*, *debug=True*)

4.2 RNA Secondary Structure

Secondary structure analysis

exception rna_tools.SecondaryStructure.**ExceptionOpenPairsProblem**

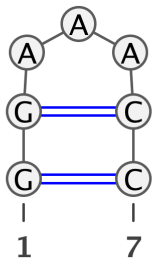
rna_tools.SecondaryStructure.**draw_ss**(*title*, *seq*, *ss*, *img_out*, *resolution=4*, *verbose=False*)

Draw Secondary Structure using VARNA (you need correct configuration for this).

If everything is OK, return None, if an error (=exception) return stderr.

Usage:

```
>>> seq = 'GGAAACC'
>>> ss =  '((...))'
>>> img_out = 'output/demo.png'
>>> draw_ss('rna', seq, ss, img_out)
>>> print('Made %s' % img_out)
Made output/demo.png
```



rna

Can be used with http://geekbook.readthedocs.io/en/latest/rna.html

rna_tools.SecondaryStructure.**parse_vienna_to_pairs**(*ss*, *remove_gaps_in_ss=False*)

Parse Vienna (dot-bracket notation) to get pairs.

Parameters

- **ss** (*str*) – secondary stucture in Vienna (dot-bracket notation) notation
- **remove_gaps_in_ss** (*bool*) – remove - from ss or not, design for DCA (tpp case `ss = "(((((((((.((((.(((.....))))))).....------).....)"` works with pk of the first level, `[[]]`

Returns

(pairs, pairs_pk)

Return type

list of two lists

Examples:

```
>>> parse_vienna_to_pairs('((..))')
([[1, 6], [2, 5]], [])

>>> parse_vienna_to_pairs('(([[))]]')
([[1, 6], [2, 5]], [[3, 8], [4, 7]])

>>> parse_vienna_to_pairs('((--))')
([[1, 6], [2, 5]], [])

>>> parse_vienna_to_pairs('((--))', remove_gaps_in_ss=True)
([[1, 4], [2, 3]], [])

>>> parse_vienna_to_pairs('((((......')
Traceback (most recent call last):
  File "/usr/lib/python2.7/doctest.py", line 1315, in __run
    compileflags, 1) in test.globs
  File "<doctest __main__.parse_vienna_to_pairs[4]>", line 1, in <module>
    parse_vienna_to_pairs('((((......')
  File "./SecondaryStructure.py", line 106, in parse_vienna_to_pairs
    raise ExceptionOpenPairsProblem('Too many open pairs (()) in structure')
ExceptionOpenPairsProblem: Too many open pairs (()) in structure
```

4.2.1 rna_dot2ct.py

The output file is <input-file>.ct

Wrapper to

RNAstructure: software for RNA secondary structure prediction and analysis. (2010). RNAstructure: software for RNA secondary structure prediction and analysis., 11, 129. http://doi.org/10.1186/1471-2105-11-129

```
usage: rna_dot2ct.py [-h] [-v] file
```

file

Input is: >seq aaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaa ((...((((((((((.....))))))))))..))

-h, --help

show this help message and exit

-v, --verbose

be verbose

4.2.2 Secondary structure format conversion

rna_convert_pseudoknot_formats

Run this as:

```
python rna-pk-simrna-to-one-line.py test_data/simrna.ss
```

Convert:

```
> a
....((.(..(((....))).((((.(.........).)))....).)).......((((......))))
.............................((((.................))))..............
```

to:

```
> a
....((.(..(((....))).((((.(..[[[[...).)))....).))...]]]](((......))))
```

and:

```
>2 chains
(((((......)))))........(.((....(.......)..(((. .)))...)).)
.....((((((....................))))))........ ..........
```

to:

```
>2 chains
(((((([[[[[)))))........(.((....(]]]]]].)..(((. .)))...)).)
```

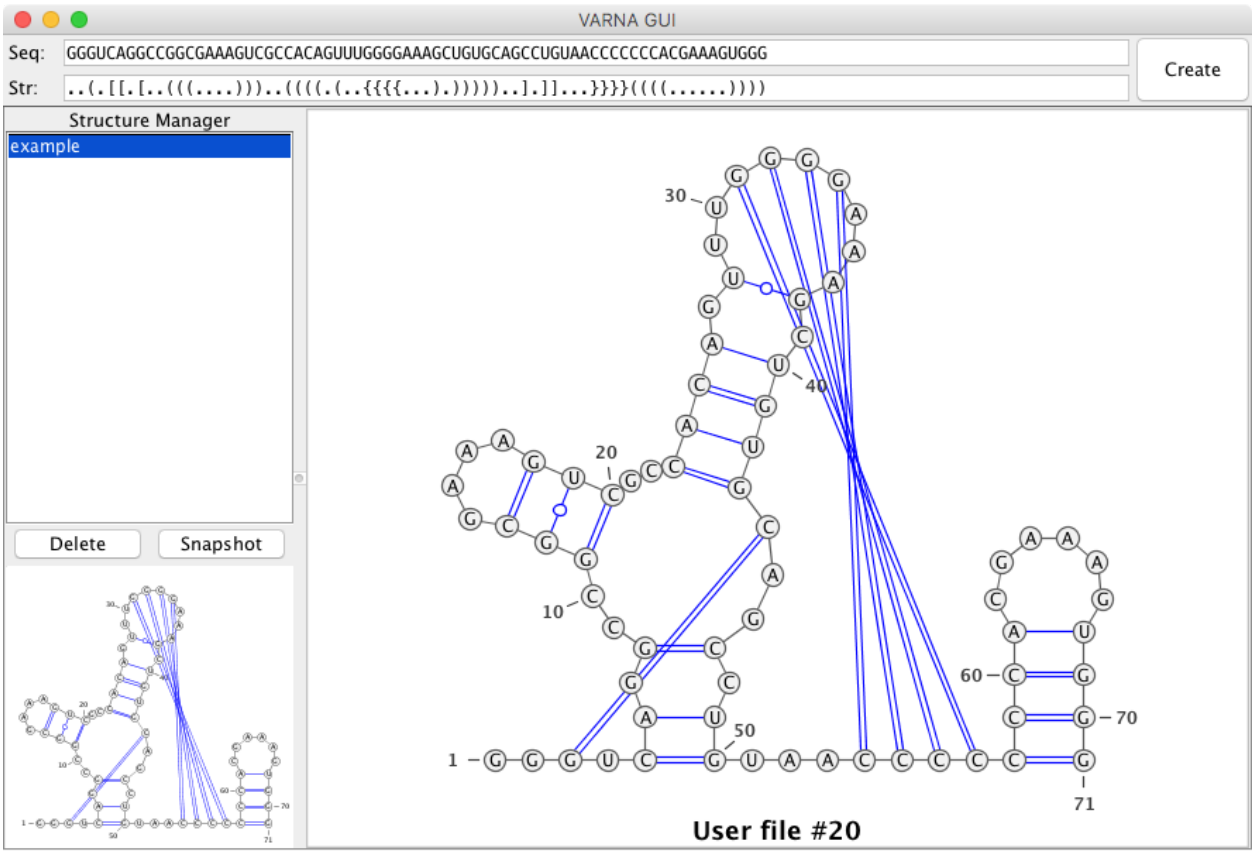
and:

```
> b
..(.......(((....))).((((.(.........).)))))..............((((......))))
....((.(.....................................).))......................
.............................((((.................))))..............
```

to:

```
> b
..(.[[.[..(((....))).((((.(..{{{{...).)))))..].]]...}}}}((((......))))
```

and it works with VARNA:



Convert a secondary structure with a pk to the SimRNA format:

```
rna_convert_pseudoknot_formats git:(master)  python rna_ss_pk_to_simrna.py test_data/ss_
↪with_pk.ss
(((((((((([)))))........(.((....[]]]]]].)..(((. .))))...)).)

(((((......)))))........(.((....(.......)..(((. .))))...)).)
.....((((((.....................))))))........ ..........
```

rna_tools.tools.rna_convert_pseudoknot_formats.rna_ss_pk_to_simrna.**get_multiple_lines**(*ss*)

rna_tools.tools.rna_convert_pseudoknot_formats.rna_ss_pk_to_simrna.**get_parser**()

rna_tools.tools.rna_convert_pseudoknot_formats.rna_ss_pk_to_simrna.**is_pk**(*ss*)

4.3 Search

4.3.1 Blast PDB

A super-simple wrapper around Blast on the PDB db (online).

class rna_tools.BlastPDB.**BlastPDB**(*seq*)

BlastPDB - run Blast online on the PDB database.

This can be used in Jupiter based RNA notebooks, e.g. https://github.com/mmagnus/rna-pdb-tools/blob/master/rp18.ipynb

Warning: getBlastPDB1 has been permanently removed as part of our announced shutdown on December 9th, 2020. https://www.rcsb.org/pdb/rest/getBlastPDB1

Usage:

```
>>> p = BlastPDB(
↪'GGGUCAGGCCGGCGAAAGUCGCCACAGUUUGGGGAAAGCUGUGCAGCCUGUAACCCCCCCACGAAAGUGGG')
>>> p.search()
>>> p.result
u'<HTML>\n<TITLE>BLAST Search Results</TITLE>...
```

Parameters
seq – string

search()
Search online the seq.

4.3.2 Rfam Search

A super-simple wrapper around cmscan (Infernal) on local Rfam database.

class rna_tools.RfamSearch.**RfamSearch**
RfamSearch (local).

Rfam is a collection of multiple sequence alignments and covariance models representing non-coding RNA families. Rfam is available on the web http://rfam.xfam.org/. The website allow the user to search a query sequence against a library of covariance models, and view multiple sequence alignments and family annotation. The database can also be downloaded in flatfile form and searched locally using the INFERNAL package (http://infernal.wustl.edu/). The first release of Rfam (1.0) contains 25 families, which annotate over 50 000 non-coding RNA genes in the taxonomic divisions of the EMBL nucleotide database.

Infernal ("INFERence of RNA ALignment") is for searching DNA sequence databases for RNA structure and sequence similarities. It is an implementation of a special case of profile stochastic context-free grammars called covariance models (CMs). A CM is like a sequence profile, but it scores a combination of sequence consensus and RNA secondary structure consensus, so in many cases, it is more capable of identifying RNA homologs that conserve their secondary structure more than their primary sequence.

Infernal *cmscan* is used to search the CM-format Rfam database.

Setup:

- download the database from ftp://ftp.ebi.ac.uk/pub/databases/Rfam/CURRENT (file: Rfam.cm.gz, ~30mb)
- install http://eddylab.org/infernal/
- set up RFAM_DB_PATH in the config file of rna-tools.
- compress Rfam.cm

Example of compressing the database:

```
$ cmpress Rfam.cm
Working...    done.
Pressed and indexed 3016 CMs and p7 HMM filters (3016 names and 3016 accessions).
Covariance models and p7 filters pressed into binary file:  Rfam.cm.i1m
SSI index for binary covariance model file:                 Rfam.cm.i1i
```

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```
Optimized p7 filter profiles (MSV part)  pressed into:      Rfam.cm.i1f
Optimized p7 filter profiles (remainder) pressed into:      Rfam.cm.i1p
```

Cite: Nawrocki and S. R. Eddy, Infernal 1.1: 100-fold faster RNA homology searches, Bioinformatics 29:2933-2935 (2013).

cmscan(*seq*, *verbose=False*)

Run cmscan on the seq.

Usage:

```
>>> seq = RNASequence("GGCGCGGCACCGUCCGCGGAACAAACGG")
>>> rs = RfamSearch()
>>> hit = rs.cmscan(seq)
>>> print(hit)
# cmscan :: search sequence(s) against a CM database...
```

Parameters
seq – string

Returns
result

Return type
string

exception rna_tools.RfamSearch.**RfamSearchError**

4.4 RNA Alignment

RNAalignment - a module to work with RNA sequence alignments.

To see a full demo what you can do with this util, please take a look at the jupiter notebook (https://github.com/mmagnus/rna-pdb-tools/blob/master/rna_tools/tools/rna_alignment/rna_alignment.ipynb)

Load an alignment in the Stockholm:

```
   alignment = ra.RNAalignment('test_data/RF00167.stockholm.sto')

or fasta format::

    import rna_alignment as ra
    alignment = ra.fasta2stokholm(alignment.fasta)
    alignment = ra.RNAalignment
```

Parameters of the aligmnent:

```
print(alignment.describe())
```

Consensus SS:

```
print(alignment.ss_cons_with_pk)
```

Get sequnce/s from teh aligment:

```
>>> seq = a.io[0]
```

4.4.1 RNASeq

class rna_tools.tools.rna_alignment.rna_alignment.**RNASeq**(*id*, *seq*, *ss=None*)

RNASeq.

Parameters

- **id** (*str*) – id of a sequence
- **seq** (*str*) – seq, it be uppercased.
- **ss** (*str*) – secondary structure, default None

seq_no_gaps

seq.replace('-', '')

Type
str

ss_no_gaps

ss.replace('-', '')

Type
str

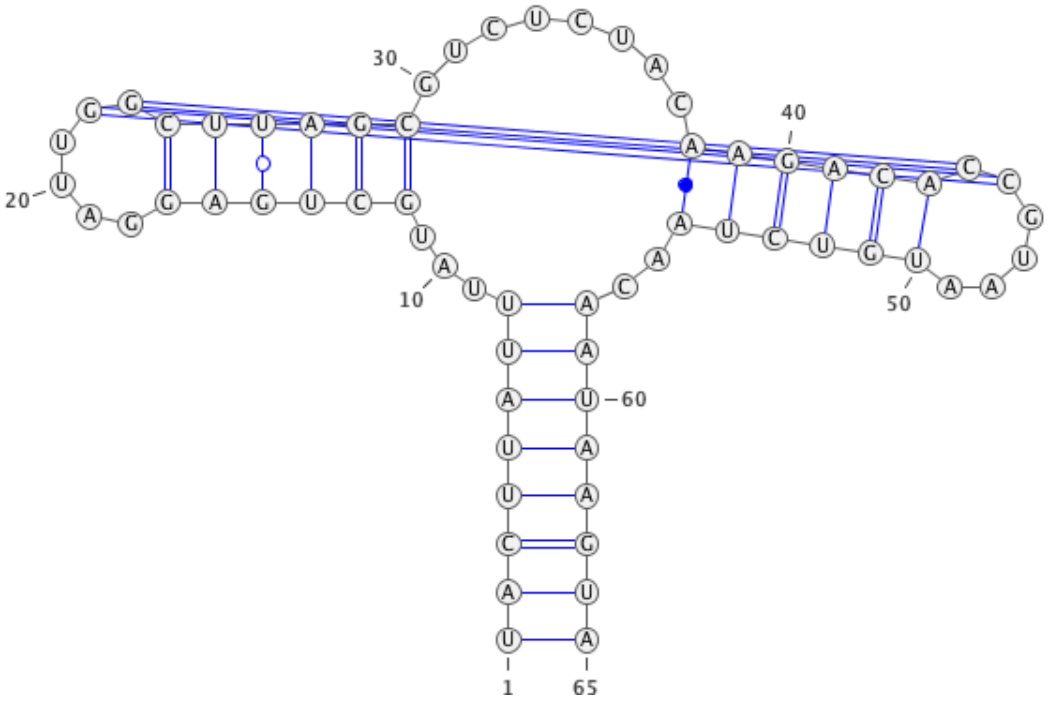
Warning:

```
>>> if 'EF' in s.id: print('Y')
Y
>>> if 'EF' in s: print('Y')
# nothing
```

draw_ss(*title=''*, *verbose=False*, *resolution=1.5*)

Draw secondary structure of RNA with VARNA.

VARNA: Visualization Applet for RNA A Java lightweight component and applet for drawing the RNA secondary structure



Cite: VARNA: Interactive drawing and editing of the RNA secondary structure Kevin Darty, Alain Denise and Yann Ponty Bioinformatics, pp. 1974-197,, Vol. 25, no. 15, 2009

http://varna.lri.fr/

get_conserved(*consensus*, *start=0*, *to_pymol=True*, *offset=0*)

Start UCGGGGUGCCCUUCUGCGUG——————————————————————AAGGC-UGAGAAAUACCCGU————————————————————-AUCACCUG-AUCUGGAU-AAUGC XXXXXXXXXXXXGXGXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX————————————————- XXXXX-XCUGAGAXXXXXXXXXXXXXXXXXXXXXX————————————————-XXXXXXXX-XXXXXXXX-ACXUG

get_distance_to(*nseq*)

Get distance of self.seq to nseq.

get_ss_std()

remove_columns(*to_remove*)

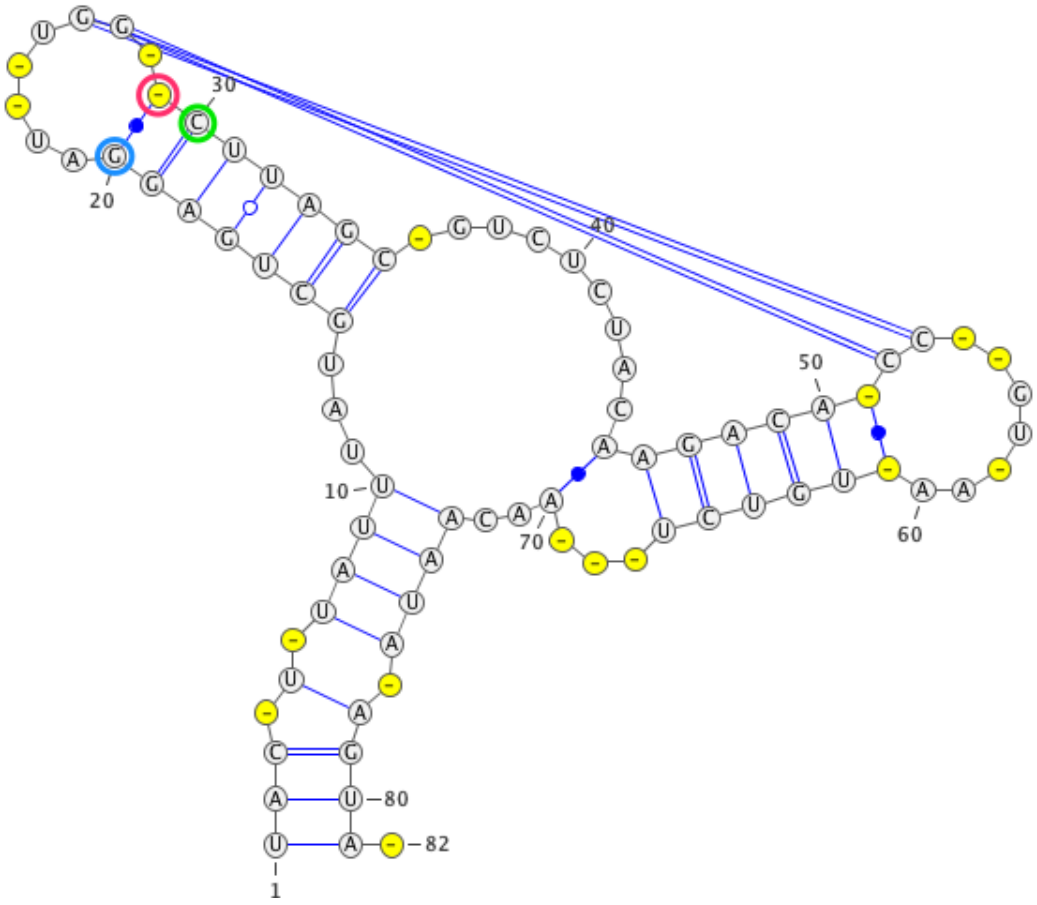
indexing from 0

remove_gaps(*check_bps=True*, *only_canonical=True*, *allow_gu=True*)

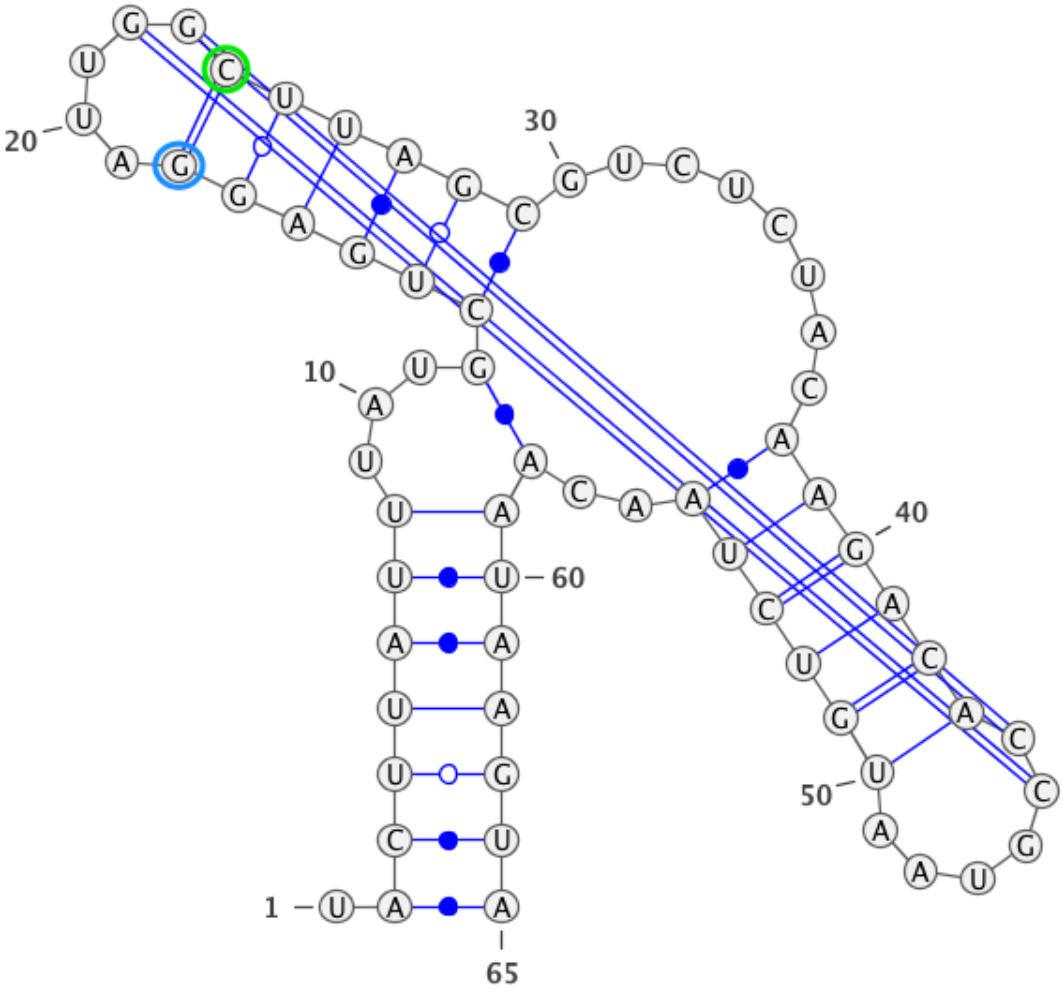
Remove gaps from seq and secondary structure of the seq.

Parameters

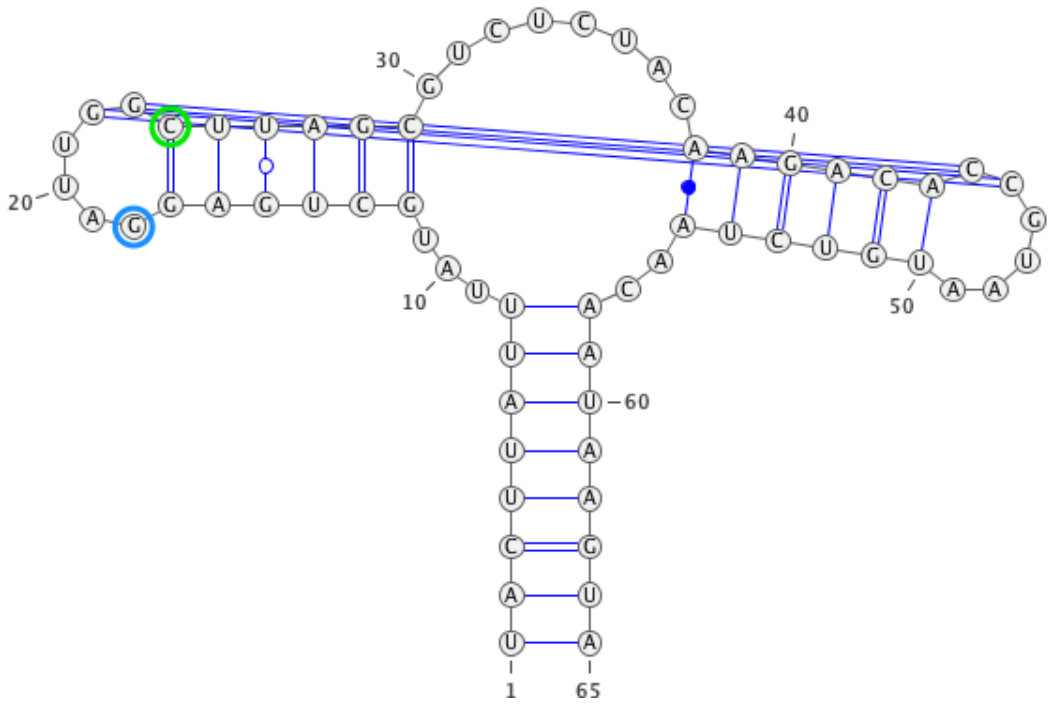
- **check_bps** (*bool*) – fix mistakes as
- **only_canonical** (*bool*) – keep in ss only pairs GC, AU
- **allow_gu** (*bool*) – keep in ss also GU pair



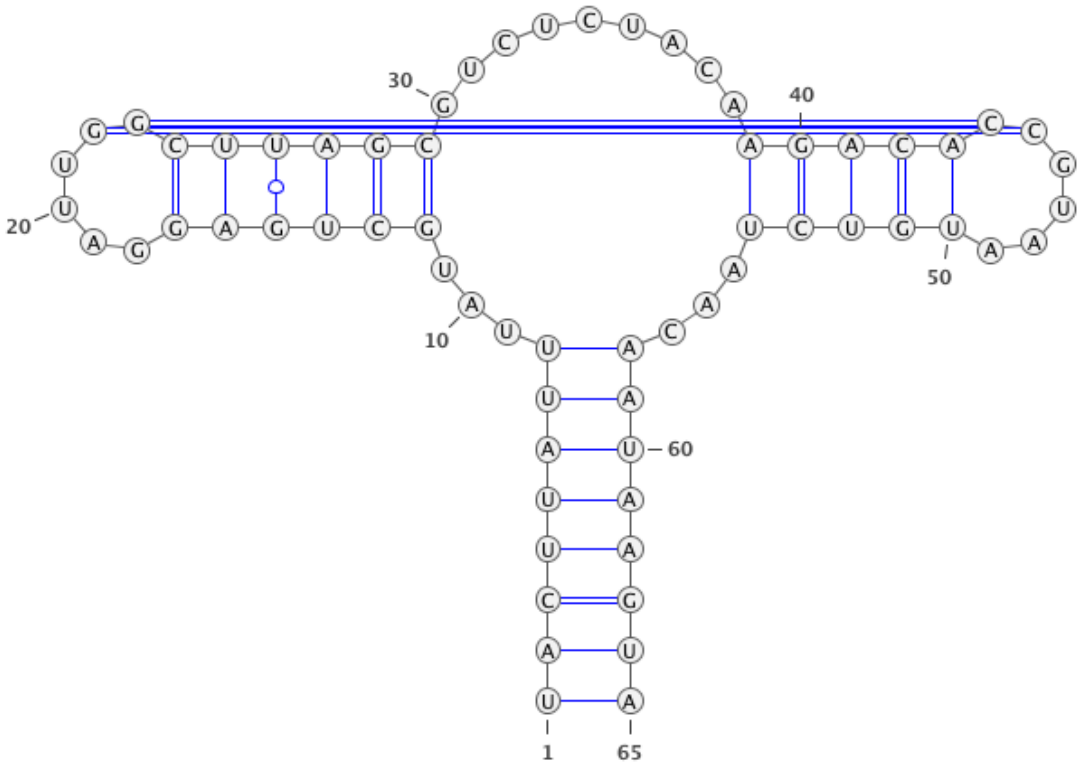
A residue “paired” with a gap.



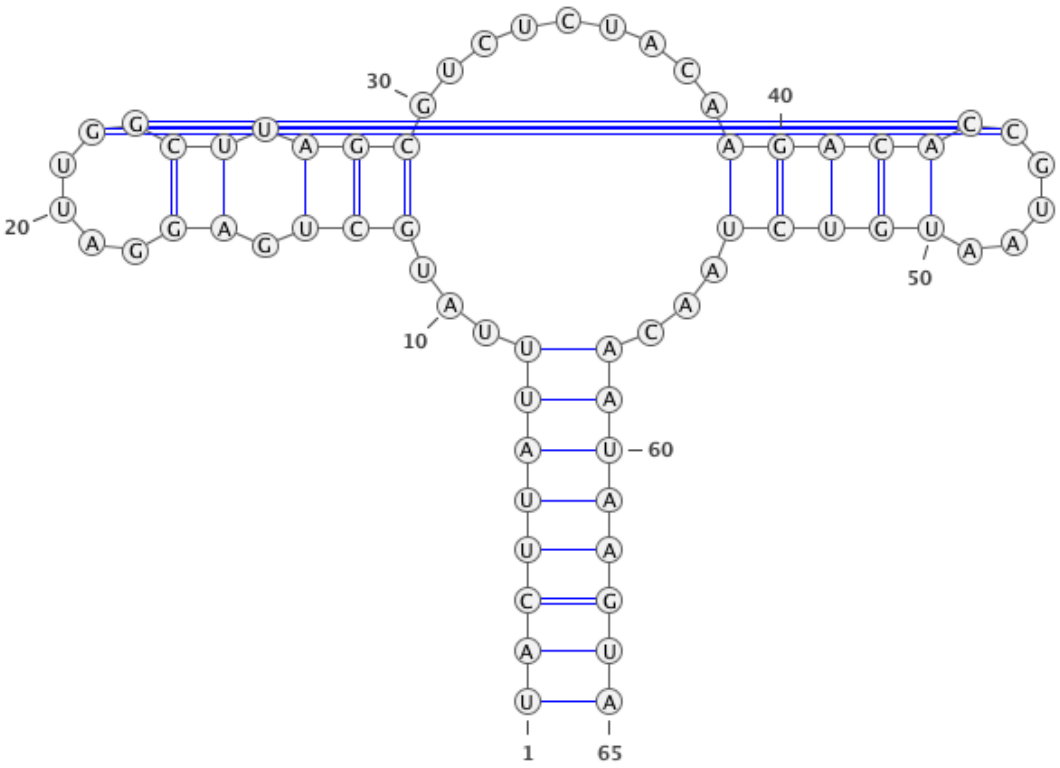
paired with any residues (in the blue circle). If yes, then this residues is unpair (in this case) -> .).



if `only_canonical` (by default) is True then only GC, AU can be paired.



If `allow_gu` is False (be default is True) then GU pair is also possible.



If you provide seq and secondary structure such as:

```
GgCcGGggG.GcggG.cc.u.aAUACAAuACCC.GaAA.GGGGAAUAaggCc.gGCc.gu......CU.......
↪uugugcgGUuUUcaAgCccCCgGcCaCCcuuuu
(((((((((....((.((............(((......)))......))))..(((.(.....................
↪))))........)))))))))........
```

gaps will be remove as well.

ss_to_bps()

Convert secondary structure into a list of basepairs.

Returns

a list of base pairs, e.g. [[0, 80], [1, 79], [2, 78], [4, 77], [6, 75], [7, 74], ...]

Return type

bps (list)

4.4.2 RNAalignment

class rna_tools.tools.rna_alignment.rna_alignment.**RNAalignment**(*fn=''*, *fetch=''*)

RNA alignment - adapter class around BioPython to do RNA alignment stuff

Usage (for more see IPython notebook https://github.com/mmagnus/rna-tools/blob/master/rna_tools/tools/rna_alignment/rna_alignment.ipynb)

```
>>> a = RNAalignment('test_data/RF00167.stockholm.sto')
>>> print(a.tail())
>>> print(a.ss_cons)
```

Parameters

- **fn** (*str*) – Filename
- **io** (*Bio.AlignIO*) – AlignIO.read(fn, "stockholm")
- **lines** (*list*) – List of all lines of fn
- **seqs** (*list*) – List of all sequences as class:*RNASeq* objects
- **rf** (*str*) – ReFerence annotation, the consensus RNA sequence

Read more:

- http://biopython.org/DIST/docs/api/Bio.AlignIO.StockholmIO-module.html

and on the format itself

- https://en.wikipedia.org/wiki/Stockholm_format
- http://sonnhammer.sbc.su.se/Stockholm.html

Warning: fetch requires urllib3

align_seq(*seq*)

Align seq to the alignment.

Using self.rf.

Parameters
seq (*str*) – sequence, e.g. `-GGAGAGUA-GAUGAUUCGCGUUAAGUGUGUGUGA-AUGGGAUGUC...`

Returns
seq that can be inserted into alignemnt, `.-.GG.AGAGUA-GAUGAUUCGCGUUA!.` -> -

Return type
str

copy_ss_cons_to_all(*verbose=False*)

copy_ss_cons_to_all_editing_sequence(*seq_id*, *before*, *after*)

Change a sequence's sec structure.

Parameters

- **seq_id** – string, sequence id to change, eg: `AE009948.1/1094322-1094400`
- **before** – string, character to change from, eg: `,`
- **after** – string, character to change to, eg: `.`

Warning: before and after has to be one character long

describe()

Describe the alignment.

> print(a.describe()) SingleLetterAlphabet() alignment with 13 rows and 82 columns

find_core(*ids=None*)

Find common core for ids.

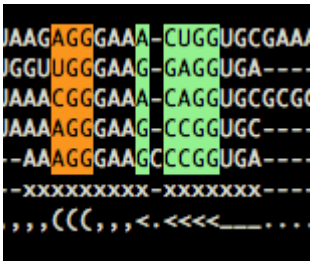


Fig. By core, we understand columns that have all homologous residues. The core is here marked by *x*.

Parameters

id – list, ids of seq in the alignment to use

find_seq(*seq*, *verbose=False*)

Find seq (also subsequences) and reverse in the alignment.

Parameters

- **seq** (*str*) – seq is upper()
- **verbose** (*bool*) – be verbose

```
seq =
↪"ggaucgcugaacccgaaaggggcgggggacccagaaaugggggcgaaucucuuccgaaaggaagaguaggguuacuccuucgacccgagcccg
↪"
hit = a.find_seq(seq, verbose=False)
ggaucgcugaacccgaaaggggcgggggacccagaaaugggggcgaaucucuuccgaaaggaagaguaggguuacuccuucgacccgagcccguca
Match: AL939120.1/174742-174619
ID: AL939120.1/174742-174619
Name: AL939120.1
Description: AL939120.1/174742-174619
Number of features: 0
/start=174742
/end=174619
/accession=AL939120.1
Per letter annotation for: secondary_structure
Seq('CCAGGUAAGUCGCC-G-C--ACCG---------------GUCA-----------...GGA',␣
↪SingleLetterAlphabet())
GGAUCGCUGAACCCGAAAGGGGCGGGGGACCCAGAAAUGGGGCGAAUCUCUUCCGAAAGGAAGAGUAGGGUUACUCCUUCGACCCGAGCCCGUCA
```

find_seq_exact(*seq*, *verbose=False*)

Find seq (also subsequences) and reverse in the alignment.

Parameters

- **seq** – string, seq, seq is upper()
- **verbose** – boolean, be verbose or not

format_annotation(*t*)

get_clean_ss(*ss*)

get_distances()

Get distances (seq identity) all-vs-all.

With BioPython.

blastn: `Bad alphabet 'U' in sequence 'AE008922.1/409481-409568' at position '7'` only for DNA?

read more (also about matrix at <http://biopython.org/wiki/Phylo> and HTTP://biopython.org/DIST/docs/api/Bio.Phylo.TreeConstruction.DistanceCalculator-class.html

get_gc_rf()

Return (str) `#=GC RF` or '' if this line is not in the alignment.

get_seq(*seq_id*)

get_seq_ss(*seq_id*)

get_seq_with_name(*seq_name*)

get_shift_seq_in_align()

RF_cons vs '#=GC RF' ???

get_ss_cons()

Returns
SS_cons_pk line or None if there is now SS_cons_pk.

get_ss_cons_pk()

Returns
SS_cons_pk line or None if there is now SS_cons_pk:

get_ss_remove_gaps(*seq*, *ss*)

Parameters

- **seq** – string, sequence
- **ss** – string, ss

UAU-AACAUAUAAUUUUGACAAUAUGG-GUCAUAA-GUUUCUACCGGAAUACC–GUAAAUAUUCU—GACUAUG-UAUA- (((.(.((((,,,(((((((_______.)))))))..,,,,,,,,(((((((__..._____)))))))...),,)))).)))).

get_the_closest_seq_to_ref_seq(*verbose=False*)

Example:

```
>>> a = RNAalignment("test_data/RF02221.stockholm.sto")
>>> a.get_the_closest_seq_to_ref_seq()
AF421314.1/431-344
```

head()

map_seq_on_align(*seq_id*, *resis*, *v=True*)

Parameters

- **seqid** – seq_id, 'CP000721.1/2204691-2204775'
- **resis** – list resis, [5,6]

maps:

```
[5, 6, 8]
CAC-U
CAC-U-
CAC-U-UA
[4, None, 6]
```

map_seq_on_seq(*seq_id*, *seq_id_target*, *resis*, *v=True*)

Parameters

- **seq_id** – seq_id, 'AAML04000013.1/228868-228953'
- **seq_id_target** – seq_id of target, 'CP000721.1/2204691-2204778'
- **resis** – list resis, [5,6]

map:

```
[4, 5, 6]
UAU-A
UAU-AA
UAU-AAC
[5, 6, 7]
CAC-U
CAC-U-
CAC-U-U
[4, None, 5]
```

plot(*plot_fn='rchie.png'*)

reload_alignment()

remove_empty_columns(*verbose=False*)

Remove empty columns in place.

Example:

```
>>> a = RNAalignment("test_data/zmp.stk")
>>> print(a)
SingleLetterAlphabet() alignment with 6 rows and 319 columns
---ACCUUGCGCGACUGGCGAAUCC-------------------...AAU CP001644.1/756294-756165
--GCUCUCGCGCGACUGGCGACUUUG------------------...GAA CU234118.1/352539-352459
UGAGUUUUCUGCGACUGACGGAUUAU------------------...CUG BAAV01000055.1/2897-2982
GCCCGUUCGCGUGACUGGCGCUAGU-------------------...CGA CP000927.1/5164264-5164343
-----GGGUCGUGACUGGCGAACA---------------------...--- zmp
UCACCCCUGCGUGACUGGCGAUA----------------------...GUU AP009385.1/718103-718202
>>> a.remove_empty_columns()
>>> print(a)
SingleLetterAlphabet() alignment with 6 rows and 138 columns
---ACCUUGCGCGACUGGCGAAUCC-UGAAGCUGCUUUG-AGCG...AAU CP001644.1/756294-756165
--GCUCUCGCGCGACUGGCGACUUUG------------------...GAA CU234118.1/352539-352459
UGAGUUUUCUGCGACUGACGGAUUAU------------------...CUG BAAV01000055.1/2897-2982
GCCCGUUCGCGUGACUGGCGCUAGU-------------------...CGA CP000927.1/5164264-5164343
-----GGGUCGUGACUGGCGAACA--------G-----------...--- zmp
UCACCCCUGCGUGACUGGCGAUA--------GAACCCUCGGGUU...GUU AP009385.1/718103-718202
```

go over all seq modifes self.nss_cons

property ss_cons_std

property ss_cons_with_pk

go over ss_cons and overwrite bp is there is pk (ss_cons_pk)

ss_cons: (((.(.((((„„(((((((_______.)))))))..„„„„„„(((((((__..._____))))))...),„)))).)))). ss_cons_pk: .....[[.....]]..... ss_cons_with_pk: (((.(.((((„„(((((((___[[__.)))))))..„„„„„„(((((((__..._]]__))))))...),„)))).)))).

"return ss_cons_with_pk: string, e.g. (((.(.((((„„(((((((___[[__.))))

property ss_cons_with_pk_std

subset(*ids*, *verbose=False*)

Get subset for ids:

```
# STOCKHOLM 1.0
#=GF WK Tetrahydrofolate_riboswitch
```

AAQK01002704.1/947-1059 -U-GC-AAAAUAGGUUUCCAUGC.. #=GC SS_cons .(.((.((—-((((((((((... #=GC RF .g.gc.aGAGUAGggugccgugc.. //

tail()

trimmed_rf_and_ss()

Remove from RF and SS gaps.

Returns
trf, tss - new RF and SS

Return type
(str,str)

write(*fn*, *verbose=False*)

Write the alignment to a file

4.4.2.1 rna_alignment_get_species.py

This is an improved version of the script that uses the Rfam MySQL database online interface (thanks @akaped for this idea) (so you need to be connected to the Internet, of course). Redirect the output to the file.

```
AB010698.1/46416-46518          GUC-CC---      Homo-sapiens-(human)/1-107                    GUG-CUCGC------
AARH01001853.1/272694-272796    GUC-UC---      Saccharomyces-cerevisiae-(baker's-yeast)/1-113 GUU-CGCGAAGUA--
X60506.1/390-492                GUC-CC---      Saccharomyces-cerevisiae-(baker's-yeast).1/1-113 GUU-CGCGAAGUA--
AC146705.11/15272-15374         GUC-CC---      Saccharomyces-cerevisiae-RM11-1a/1-113        GUU-CGCGAAGUA--
AASG02002949.1/2307-2409        GUC-CC---  vs  Schizosaccharomyces-pombe-(fission-yeast)/1-153 UGA-UC---------
AACV01009611.1/38269-38371      GUC-CC---      -/1-0                                         ---------------
AAAA02013555.1/2292-2394        GUC-CC---      Aedes-aegypti-(yellow-fever-mosquito)/1-107    GUC-UUUGC------
CR855100.1/43897-43999          GUC-CC---      Aegilops-tauschii/1-105                       GUC-CN---------
```

Warning: This scripts needs mysql-connector-python-rf module to connect the Rfam MySQL server, so install it before using: `pip install mysql-connector-python-rf`.

Example:

```
$ rna_alignment_get_species.py RF00004.stockholm.stk
# STOCKHOLM 1.0
Sorex-araneus-(European-shrew)                      AUCGCU-UCU----CGGCC--UUU-U
```

Examples 2:

```
$ rna_alignment_get_species.py u5_rfam_u5only.stk --verbose
# STOCKHOLM 1.0
#=GF WK U5_spliceosomal_RNA
#=GF NC 39.90
#=GF RT The spliceosomal snRNAs of Caenorhabditis elegans.
#=GF TC 40.00
#=GF RN [3]
(...)
#=GF AC RF00020
#=GF SE Zwieb C, The uRNA database, PMID:9016512; PMID:18390578
#=GF GA 40.00
#=GF BM cmbuild -F CM SEED
#=GF TP Gene; snRNA; splicing;
Bos-taurus-(cattle)                                 GAUC-GUAUAAAUCUUUCGCCUUUUACUAAAGA-
↪UUUCCG----UGG-A--GA-G
Sorex-araneus-(European-shrew)                      GAUC-GUAUAAAUCUUUCGCCUUUUACUAAAGA-
↪UUUCCG----UGG-A--GA-G
Ictidomys-tridecemlineatus-(thirteen-lined-ground- GAUC-GUAUAAAUCUUUCGCCUUUUACUAAAGA-
↪UUUCCG----UGG-A--GA-G
Monodelphis-domestica-(gray-short-tailed-opossum)  GAUC-GUAUAAAUCUUUCGCCUUUUACUAAAGA-
↪UUUCCG----UGG-A--GA-G
Oryctolagus-cuniculus-(rabbit)                      GAUC-GUAUAAAUCUUUCGCCUUUUACUAAAGA-
↪UUUCCG----UGG-A--GA-G
Cavia-porcellus-(domestic-guinea-pig)               GAUC-GUAUAAAUCUUUCGCCUUUUACUAAAGA-
↪UUUCCG----UGG-A--GA-G
Ochotona-princeps-(American-pika)                   GAUC-GUAUAAAUCUUUCGCCUUUUACUAAAGA-
↪UUUCCG----UGG-A--GA-G
```

```
usage: rna_alignment_get_species.py [-h] [-v] [--debug] [--id-width ID_WIDTH]
                                    [--evo-mapping EVO_MAPPING]
                                    [--evo-mapping-default] [--one]
                                    [--osfn OSFN] [--rfam]
                                    alignment
```

alignment

alignment

-h, --help

show this help message and exit

-v, --verbose

be verbose

--debug

--id-width <id_width>

define width of ids, trim species name when longer than this

--evo-mapping <evo_mapping>

--evo-mapping-default

--one

--osfn <osfn>

cache file

--rfam

4.4.2.2 rna_alignment_calc_energy.py

Calculate energy (.cet) format:

```
UGGC-CCCUGCGCAA-GGAUGACA
(((..((((.....).)).)..)))).
(((..(((((***)).)).)..))))
```

Examples:

```
 $ rna_alignment_calc_energy.py --template alignments/u6-lower.cet alignments/u6-only-
↪RemovedGapped.stk -v
       --loop-upper guaa --loop-lower guaa
       --loop-upper-cst '(..)' --loop-lower-cst '(..)'
 calc-energy2.py --template u6atac-template.txt u6atac_u6only.sto -v
./calc-energy2.py --template alignments/u6-lower.cet --one alignments/u6-lower-stem-only.
↪sto
```

Takes cet files (calc-energy-templets):

```
$ rna_alignment_calc_energy.py --template test_data/u6-lower.cet --one test_data/u6-only.
↪stk  -v # --loop-seq test_data/u6-only-loop-seq-u6-lower
N/A% (0 of 182) |                                                                    ␣
↪                                                  | Elapsed Time: 0:00:00 ETA:  --:--
↪:--=============================================================================
AB010698.1/46467-46488
(((..((((.....).)).)..)))).
UGGC-CCCUGCGCAA-GGAUGACA
lower -------------------------------------
UGG ugcgca ACA
(((******)))
UGGugcgcaACA
(((((..))))) -10.64
upper -------------------------------------
UGGC-CCCUGCGCAA-GGAUGACA
CCC ugcgca AGG
CCCugcgcaAGG
(((((..))))) -9.6
                       id  low_energy       low_seq        low_ss  up_energy        up_
↪seq         up_ss
0  AB010698.1/46467-46488      -10.64  UGGugcgcaACA  (((((..)))))       -9.6 ␣
↪CCCugcgcaAGG  (((((..)))))
Done: u6-only-loop-seq-u6-lower
```

by parsing output from MC-Sym:

```
domains have 5451 elements.
 10:47:16 up 141 days, 26 min,  0 users,  load average: 1.45, 1.30, 1.56
Score: -999.000 GAACAUGGUUCUUGCCUUUUACCAGAACCAUCCGGGUGUUG
Total number of MB structures with 3 stems: 16041
(overlaps: 0, !energy: 335585)
</pre><P><H2>Sorting the structures...
<P></H2><pre></pre><H2><P><P><P>Filtered and Sorted solutions:<P><P><P></H2><pre>
</pre><H2><P><P><P><a HREF="http://biwww2.informatik.uni-freiburg.de/Software/MARNA/
↪index.html" target="_blank">MARNA</a>-formatted:<P><P><P></H2><pre>
GAACAUGGUUCUUGCCUUUUACCAGAACCAUCCGGGUGUUG
((((((((((..))))))))))(((((((...))))))) -33.20 ( -0.69)
((((((((((....))))))))))(((((((...))))))) -33.17 ( -0.69)
((((((((((((((...))))))))))))).....)))) -32.40 ( +0.00)

Backtracking with 2 variables (stems):
domains have 5451 elements.
 10:47:16 up 141 days, 26 min,  0 users,  load average: 1.45, 1.30, 1.56
Score: -999.000 GAACAUGGUUCUUGCCUUUUACCAGAACCAUCCGGGUGUUG
Total number of MB structures with 2 stems: 9555
(overlaps: 0, !energy: 165582)
</pre><P><H2>Sorting the structures...
<P></H2><pre></pre><H2><P><P><P>Filtered and Sorted solutions:<P><P><P></H2><pre>
</pre><H2><P><P><P><a HREF="http://biwww2.informatik.uni-freiburg.de/Software/MARNA/
↪index.html" target="_blank">MARNA</a>-formatted:<P><P><P></H2><pre>
GAACAUGGUUCUUGCCUUUUACCAGAACCAUCCGGGUGUUG
((((((((((..))))))))))(((((((...))))))) -33.20 ( -0.69)
((((((((((....))))))))))(((((((...))))))) -33.17 ( -0.69)
((((((((((((((...))))))))))))).....)))) -32.40 ( +0.00)
```

```
usage: rna_alignment_calc_energy.py [-h] [--debug] [--one] [--method METHOD]
                                    [--csv CSV] [--loop-seq]
                                    [--template TEMPLATE] [--flanks FLANKS]
                                    [-v]
                                    alignment
```

alignment
: an alignment in the Stockholm format

-h, --help
: show this help message and exit

--debug

--one
: one only for the first seq

--method <method>
: mcfold or rnastructure_CycleFold

--csv <csv>

--loop-seq

--template <template>

--flanks <flanks>

GC be default

-v, --verbose

4.4.2.3 rna_align_get_ss_from_fasta.py

Input as a file:

```
>ade
GCU-U-CAUAUAAUCCUAAUGAUAUGG-UUUGGGA-GUUUCUACCAAGAG-CC--UUAAA-CUCUU---GAUUAUG-AAGU-
(((.(.((((,,(((((((_______.)))))))..,,,,,,,,(((((((__.._____))))))...),,))))).)))).
```

to get:

```
>ade
GCUUCAUAUAAUCCUAAUGAUAUGGUUUGGGAGUUUCUACCAAGAGCCUUAAACUCUUGAUUAUGAAGU
(((((((...(((((((.......)))))))........((((((.......))))))..)))))))
```

```
usage: rna_align_get_ss_from_fasta.py [-h] file
```

file

subsection of an alignment

-h, --help

show this help message and exit

4.4.2.4 rna_align_get_ss_from_stk.py

Process an alignment in the Stockholm format to get sequences and secondary structures:

Example:

```
$ rna_align_get_ss_from_stk.py aligns/gmp_RF01786.stockholm_p75_pk.sto
AAOX01000007.1/31274-31356
AAGAAUAUAGAACACUGUGAUGAGCGGUUUUUAUUUGCACUUUAAACCGCUUGGAGUGACUAGUGCAGCCGGCCAAUGAUCUA
.(((.(((.(..(((......(((((((.............)))))))...)))..............).))).))).
CP000724.1/3560727-3560809
AAAAAUGUAGAGCAAAUGAACUGCAGGUAUACAUGGACGCCUUAAACUGCAGGGAUGUAGUGGCGUAACCGACUAACAAUAUU
((.(.(((((.(((......((((((.(......[[...[....).))))))...)))...]...]..]...))).)).).))
AACY023761929.1/1009-1091
AUAAUUUGGUGGGCGUUGAUGUGCCCUUUGUAUCUGGUCGCUUGAGGGGUACGGAGCCAAUAGCGAAACCGCCGCCGUCAUAG
.((...(((((((((......(((((((.......[.[......)))))))...)))......]...]...)))))...)).
```

```
usage: rna_align_get_ss_from_stk.py [-h] file
```

file

subsection of an alignment

-h, --help

show this help message and exit

4.4.2.5 rna_align_distance_to_seq.py

Calculate

“Process an alignment in the Stockholm format to get sequences and secondary structures:

Example:

```
$ rna_align_distance_to_seq.py test_data/gmp_ref.sto test_data/gmp_ref_distance.csv

   distance                            id
0      1.00                           gmp
1      0.69    AE000513.1/1919839-1919923
2      0.73      BA000004.3/387918-388001
3      0.69  ABFD02000011.1/154500-154585
4      0.73      AE015927.1/474745-474827
5      0.75                AAWL01000006.1
6      0.72                    AM180355.1
7      0.72      CP001116.1/102374-102457
8      0.65    AJ965256.1/1260708-1260792

                                                   seq
0  -----GCGCGGAAAC-AAUGAUGAAU--GGG-UUUA-AAUUGGGC-...
1  CUGUCGAAGAGACGC-GAUGAAUCCC--GCC-CUGUAAUUCGGGC-...
2  AAUCAAUAGGGAAGC-AACGAAGCAU--AGC-CUUU-AUAUGGAC-...
3  AAAUAUUAUAGAGAU-GUUGAAGUAU--AUU-CUAUUA-UUGGGC-...
4  AUUUUAAGAGGAAAU-UUUGAACUAU--AUA-CUU--AUUUGGGC-...
5  --UGCAA-UGGGUGU-GAUGAAGUCC--GGA-CAGUAAUGUGGGC-...
6  AAUAUUU-UAGAAAC-UGAGAAGUAU--AUC-UUAUUA-UUGGGC-...
7  AUAACGGCACGAAGC-AAUGAAAUGU--UCG-AUGU-AACCGGGC-...
8  AAAUUAAGGGGAAGC-GUUGAGCCGC--UAC-CCAU-AUGUGGUUC...

                                                   ss:
0  ((((((((((.(((.......((((..(((.(.............
1  ((((((((((.(((.......((((..(((.(.............
2  ((((((((((.(((.......((((..(((.(.............
3  ((((((((((.(((.......((((..(((.(.............
4  ((((((((((.(((.......((((..(((.(.............
5  ((((((((((.(((.......((((..(((.(.............
6  ((((((((((.(((.......((((..(((.(.............
7  ((((((((((.(((.......((((..(((.(.............
8  ((((((((((.(((.......((((..(((.(.............
```

```
usage: rna_align_distance_to_seq.py [-h] file output
```

file
: an alignment in the Stokholm format, the first seq will be used to calculate distance to (#TODO pick any seq)

output
: csv pandas file

-h, --help
: show this help message and exit

4.4.2.6 rna_align_foldability.py

Calculate statistics of foldability on an alignment.

The tool uses ENTRANA [1] to calculate, what the authors called, foldability (column: "foldability") of a given sequence into a given secondary structure.

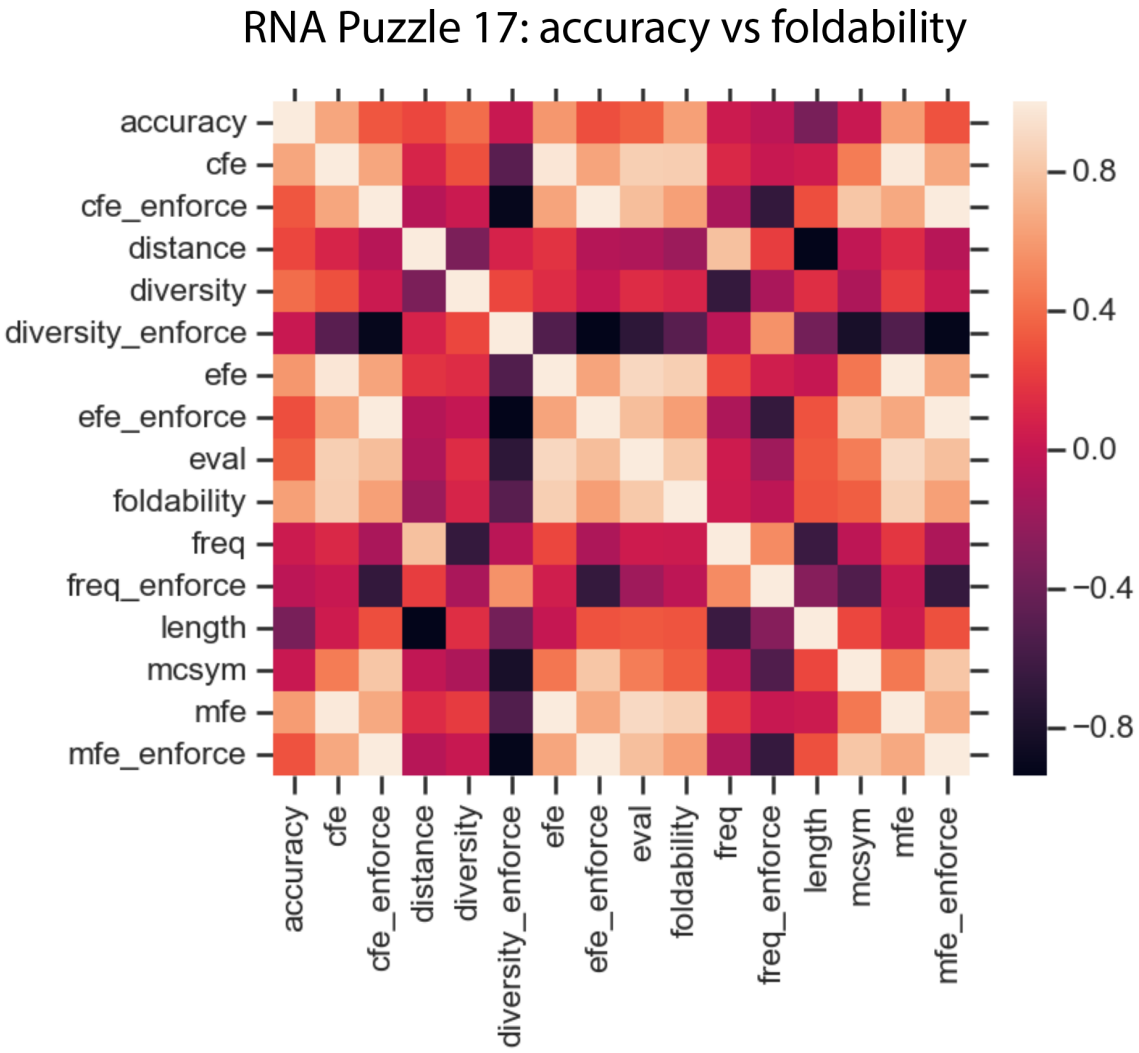
Next, MC-Fold [2] is executed to calculate free energy (column: "mcsym") on the sequence and the secondary structure obtained based on the alignment. The secondary structure is used as constraints.

The third used program is RNAfold from the Vienna package [3]. Also, in this case the secondary structure obtained with rna-tools from the RNA alignment is used as constraints, columns: "mfe" (minimum free energy), "mfess" (secondary structure for minimum free energy state), "cfe" (minimum free energy of centroid), "cfess" (secondary structure for centroid, "diversity" (ensemble diversity), "efe" (free energy of the thermodynamic ensemble), "efess" (secondary structure for the thermodynamic ensemble), "freq" (frequency of mfe structure in ensemble). RNAfold is also executed in with "–enforceConstraint" where the constraints are enforced. This run gives analogous values as the default RNAfold, to all RNAfold column "_enforce" is added.

The tool is able to calculate the distance Levenshtein (the difference between the two sequences)(column: "distance") from the target sequence and all sequence in the alignment to test if there is a bias in the accuracy towards the most similar sequences.

Another tool used from the Vienna package is RNAeval. The tool calculates free energy for a given sequence and secondary structure.

The accuracy is expressed as the median of core RMSD of 10% the lowest core RMSD models for the given sequences.



The correlations:

```
accuracy             1.000000
cfe                  0.653813
foldability          0.622038
mfe                  0.607340
efe                  0.585077
diversity            0.404350
eval                 0.349499
cfe_enforce          0.311744
mfe_enforce          0.302973
efe_enforce          0.280929
distance             0.256870
freq                 0.037037
diversity_enforce    0.018429
mcsym                0.017533
freq_enforce        -0.037991
length              -0.340809
```

The data:

We tested correlations between the above-mentioned statistics, and the highest correlation, 0.65 () was achieved to the centroid free energy calculated with RNAFold, which suggests that to some extent this metric could be used to pick sequence from the alignment to pick sequences that are more likely to fold.

However, this needs further investigation and the detailed analysis an all cases and more folded sequences.

1. Su C, Weir JD, Zhang F, Yan H, Wu T. ENTRNA: a framework to predict RNA foldability. BMC Bioinformatics. BioMed Central 2019
2. Parisien M, Major F. The MC-Fold and MC-Sym pipeline infers RNA structure from sequence data. Nature 2008;452:51-5
3. Lorenz R, Bernhart SH, Honer Zu Siederdissen C, Tafer H, Flamm C, Stadler PF, et al. ViennaRNA Package 2.0. Algorithms Mol Biol. BioMed Central; 2011;6:26-14.

Example:

```
$ python rna_align_foldability.py test_data/gmp_ref.sto test_data/gmp_foldability.csv
                                      cfess_enforce  distance  diversity
0  ((((((.(((......(((((((((..............)))))))...      1.00       3.96
1  (((.(((((((..((......(((((.(((((.......)))).......      0.69       5.56
2                                                           0.73       3.84
3                                                           0.69       5.92
4  (((....((((.((((((...(((((((.................))...      0.73       7.49
5  ((((.(((.(((..((..(((((((.................)))...      0.75       7.92
6  .(((((((((.((((.....(((((((((.................))...      0.72       5.83
7                                                           0.72       7.35
8  ...(((((((((.(((......((((((.((....(((...)))..)...      0.65       4.86

   diversity_enforce    efe  efe_enforce
0               2.89 -14.77       -13.75
1               3.70 -19.52       -18.25
2               0.00 -15.41         0.00
3               0.00 -13.55         0.00
4               2.46  -8.58        -6.91
5               6.37 -20.72       -20.08
6               2.92 -11.87       -11.38
7               0.00 -14.59         0.00
8               3.83 -21.16       -20.64

                                              efess
0  ((((((..........(((((((((..............)))))))...
1  {{..(((((((..((......(((((.(({{(.......}})).......
2  .......((((.(((..(...(((((((((..............))...
3  .....((((((.(((.....(((((((((.......{{...,}..,...
4  .......{(((.,{{{{,...(((((((((.................))...
5  {(((.(((.(((..((..(((((((((,{{...,.....)}}..)))...
6  .(((((((((.((((.....(((((((((.................))...
7  .....{,.{{{.(((......((((((((((...........,.}))...
8  ...{(((((((.(((......((((((.((....(((...)))..)...

                        ...                          length   mcsym
0                       ...                            75.0  -39.73
1                       ...                            85.0  -37.89
```

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```
2                        ...                             84.0  -35.40
3                        ...                             86.0  -36.11
4                        ...                             83.0  -37.37
5                        ...                             80.0  -43.59
6                        ...                             84.0  -42.95
7                        ...                             84.0  -36.55
8                        ...                             85.0  -43.58

                      mcsym comment
0  energy best dynamics programming
1                         BP energy
2                         BP energy
3                         BP energy
4  energy best dynamics programming
5  energy best dynamics programming
6  energy best dynamics programming
7                         BP energy
8  energy best dynamics programming

                                              mcsym ss   mfe mfe_enforce
0  ((((((.(((......(((((((.................)))))))... -13.9       -12.9
1  (((.(((((((..((......(((((.((..................... -18.0       -17.3
2  ....(..((((.(((......(((((((.................)... -14.0         0.0
3  .(...((((((.(((......(((((((..................... -12.0         0.0
4  (((....((((.(((......(((((((.............))...  -7.2        -6.1
5  ((((.(((.(((......(((((((.................)))... -18.6       -18.6
6  .(((((((((.(((......(((((((.................)... -10.5       -10.5
7  ...(.((.(((.(((......(((((((.................)... -12.8         0.0
8  ...(((((((.(((......((((((.(..................... -19.8       -19.8

                                                 mfess
0  ((((((..........(((((((((..............)))))))...
1  ((..(((((((..((......(((((.(((((.......)))).......
2  .......((((.(((......(((((((((..............))...
3  .....((((((.(((.....(((((((((.....................
4  ......................(((((((.............))...
5  ((((.(((.(((..((..((((((((((.........)))..)))...
6  .(((((((((.((((.....(((((((((.............))...
7  .....((.(((.(((......((((((((((............)))...
8  ...(((((((.(((......((((((.((....(((...)))..)...

                                           mfess_enforce
0  ((((((.(((......(((((((((..............)))))))...
1  (((.(((((((..((......(((((.(((((.......)))).......
2                                                error
3                                                error
4  (((....((((.((((((...(((((((.............))...
5  ((((.(((.(((..((..((((((((((.........)))..)))...
6  .(((((((((.((((.....(((((((((.............))...
7                                                error
8  ...(((((((.(((......((((((.((....(((...)))..)...
```

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```
                                                    seq
0  GCGCGGAAACAAUGAUGAAUGGGUUUAAAUUGGGCACUUGACUCAU...
1  CUGUCGAAGAGACGCGAUGAAUCCCGCCCUGUAAUUCGGGCACCUC...
2  AAUCAAUAGGGAAGCAACGAAGCAUAGCCUUUAUAUGGACACUUGG...
3  AAAUAUUAUAGAGAUGUUGAAGUAUAUUCUAUUAUUGGGCACCUUA...
4  AUUUUAAGAGGAAAUUUUGAACUAUAUACUUAUUUGGGCACUUUGU...
5  UGCAAUGGGUGUGAUGAAGUCCGGACAGUAAUGUGGGCACUUAGUC...
6  AAUAUUUUAGAAACUGAGAAGUAUAUCUUAUUAUUGGGCAUCUGGA...
7  AUAACGGCACGAAGCAAUGAAAUGUUCGAUGUAACCGGGCACCUAU...
8  AAAUUAAGGGGAAGCGUUGAGCCGCUACCCAUAUGUGGUUCACUCG...

                                                     ss
0  ((((((.(((......(((((((.................))))))...
1  (((.(((((((..((......(((((.((.....................
2  ....(..((((.(((......(((((((.................)...
3  .(...((((((.(((......(((((((.....................
4  (((....((((.(((......(((((((.................))...
5  ((((.(((.(((......(((((((.................)))...
6  .(((((((((.(((......(((((((.................)...
7  ...(.((.(((.(((......(((((((.................)...
8  ...(((((((.(((......((((((.(.....................

[9 rows x 26 columns]
```

```
usage: rna_align_foldability.py [-h] [--all-stars] [--dev] [--skip-mcfold]
                                [-v]
                                file output
```

file

an alignment in the Stokholm format, the first seq will be used to calculate distance to (#TODO pick any seq)

output

csv pandas file

-h, --help

show this help message and exit

--all-stars

this takes usully super long

--dev

--skip-mcfold

-v, --verbose

be verbose

4.4.3 Random assignment of nucleotides

4.4.3.1 random_assignment_of_nucleotides.py

random_assignment_of_nucleotides.py - Random assignment of nucleotides for non-typical characters in the sequence alignment (arg –alignfn or fasta file with sequneces (arg –seqfn)

```
R = G A (purine)
Y = U C (pyrimidine)
K = G U (keto)
M = A C (amino)
S = G C (strong bonds)
W = A U (weak bonds)
B = G U C (all but A)
D = G A U (all but C)
H = A C U (all but G)
V = G C A (all but T)
N = A G C U (any)
```

author: A. Zyla - azyla

Warning: Tested only on fasta files! and requires Biopython (tested with v1.68)

```
usage: random_assignment_of_nucleotides.py [-h] [-v] [--alignfn ALIGNFN]
                                           [--seqfn SEQFN] [--outfn OUTFN]
```

-h, --help
show this help message and exit

-v, --verbose
increase output verbosity

--alignfn <alignfn>
alignment in the Fasta format

--seqfn <seqfn>
sequences in the Fasta format

--outfn <outfn>
output aln file (default: alnfn .fasta -> _out.fasta)

random_assignment_of_nucleotides.py - Random assignment of nucleotides for non-typical characters in the sequence alignment (arg –alignfn or fasta file with sequneces (arg –seqfn)

```
R = G A (purine)
Y = U C (pyrimidine)
K = G U (keto)
M = A C (amino)
S = G C (strong bonds)
W = A U (weak bonds)
B = G U C (all but A)
D = G A U (all but C)
H = A C U (all but G)
```

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```
V = G C A (all but T)
N = A G C U (any)
```

author: A. Zyla - azyla

Warning: Tested only on fasta files! and requires Biopython (tested with v1.68)

rna_tools.tools.rna_alignment.random_assignment_of_nucleotides.**get_align**(*alignfn*)

Get seq from an alignment with gaps.

Args:
alignfn (str): a path to an alignment

Usage::

```
>>> get_align('test_data/aln1.fasta')
SingleLetterAlphabet() alignment with 2 rows and 13 columns
AGGGGGACAGNYU 1
CYGA------CGG 2
```

obj1', description='obj1', dbxrefs=[]), id='<unknown id>', name='<unknown name>', description='<unknown description>', dbxrefs=[])

Returns:
alignment

rna_tools.tools.rna_alignment.random_assignment_of_nucleotides.**get_parser**()

rna_tools.tools.rna_alignment.random_assignment_of_nucleotides.**get_sequences**(*seqfn*)

Get seq from an fasta file. :param seqfn: a path to a fasta file :type seqfn: str

Usage::

```
>>> get_align('test_data/fasta.fasta')
```

Returns
[SeqRecord(seq=Seq('GGGYYGCCNRW', SingleLetterAlphabet()), id='1', name='1', description='1', dbxrefs=[]), SeqRecord(seq=Seq('GGRGYYGCCUURWAA', SingleLetterAlphabet()), id='1', name='1', description='1', dbxrefs=[])]

rna_tools.tools.rna_alignment.random_assignment_of_nucleotides.**write_align**(*align*, *outfn*)

Write cleaned alignment with Biopython. :param align: a cleaned alignment :type align: obj :param outfn: a path to a new alignment file :type outfn: str

Returns
writes to a file in fasta format

Return type
none

rna_tools.tools.rna_alignment.random_assignment_of_nucleotides.**write_seq**(*seqfn*, *outfn*)

Write cleaned alignment with Biopython. :param align: a cleaned alignment :type align: obj :param outfn: a path to a new alignment file :type outfn: str

Returns
writes to a file in fasta format

Return type
none

4.4.4 CMAlign

class rna_tools.tools.rna_alignment.rna_alignment.**CMAlign**(*outputfn=None*)

CMAalign class around cmalign (of Inferal).

cmalign - aligns the RNA sequences in <seqfile> to the covariance model (CM) in <cmfile>. The new alignment is output to stdout in Stockholm format.

Example:

```
cma = ra.CMAlign()
cma.run_cmalign("ade_seq.fa", "RF00167.cm")
seq = cma.get_seq()
print 'cma hit  ', seq
print 'seq      ', a.align_seq(seq)
print 'a.rf     ', a.rf

cmd cmalign -g RF00167.cm ade_seq.fa

# STOCKHOLM 1.0
#=GF AU Infernal 1.1.2

ade          -----------------CGCUUCAUAUAAUCCUAAUGAUAUGGUUUGGGAGUUUCUACCAAGAG-
↪CCUUAAA-CUCUUGAUUAUGAAGUGA------------
#=GR ade PP  .................99**********************************************.
↪*******.***************999............
#=GC SS_cons ::::::::::::::::::(((((((,,,<<<<<<<_______>>>>>>>,,,,,,,,<<<<<<<_______
↪>>>>>>>,,)))))))):::::::::::::::
#=GC RF      ␣
↪aaaaaauaaaaaaaauucccuCgUAUAAucccgggAAUAUGGcccgggaGUUUCUACCaggcagCCGUAAAcugccuGACUAcGagggaaauuuuuu
//
cma hit    -----------------CGCUUCAUAUAAUCCUAAUGAUAUGGUUUGGGAGUUUCUACCAAGAG-CCUUAAA-
↪CUCUUGAUUAUGAAGUGA------------
seq        -----------------CGCU-U-CAUAUAAUCCUAAUGAUAUGG-UUUGGGA-GUUUCUACCAAGAG-CC--
↪UUAAA-CUCUU---GAUUAUG-AAGUGA-------------
a.rf       aaaaaauaaaaaaaauuccc.u.CgUAUAAucccgggAAUAUGG.cccggga.GUUUCUACCaggcagCC..
↪GUAAAcugccu...GACUAcG.agggaaauuuuuuuuuuu.
```

Install http://eddylab.org/infernal/

Cite: Nawrocki and S. R. Eddy, Infernal 1.1: 100-fold faster RNA homology searches, Bioinformatics 29:2933-2935 (2013).

get_gc_rf()

Get #=GC RF.

Variables
self.output – string

get_seq()

Variables
self.output – output of cmalign, string

run_cmalign(*seq*, *cm*, *verbose=True*)

Run cmalign and process the result.

Parameters

- **seq** – seq string
- **cm** – cm fn

Run:

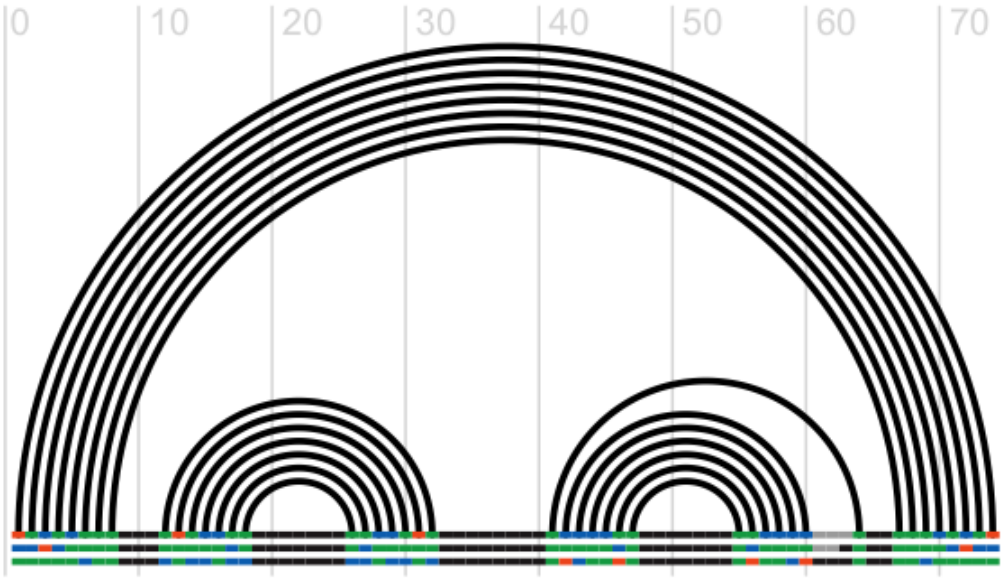
```
$ cmalign RF01831.cm 4lvv.seq
# STOCKHOLM 1.0
#=GF AU Infernal 1.1.2

4lvv         -GGAGAGUA-GAUGAUUCGCGUUAAGUGUGUGUGA-AUGGGAUGUCG-UCACACAACGAAGC---
↪GAGA---GCGCGGUGAAUCAUU-GCAUCCGCUCCA
#=GR 4lvv PP .********.******************9999998.**********.8999999******8...
↪5555...8**************.************
#=GC SS_cons (((((----((((((((((,,,,,<<-<<<<<<<<<___________>>>>>>>>>>,,,<<<<___
↪___>>>>,,,))))))))))-------)))))
#=GC RF      ␣
↪ggcaGAGUAGggugccgugcGUuAAGUGccggcgggAcGGGgaGUUGcccgccggACGAAgggcaaaauugcccGCGguacggcaccCGCAU
//
```

Warning: requires cmalign to be set in your shell

4.4.5 RChie

class rna_tools.tools.rna_alignment.rna_alignment.**RChie**

RChie - plotting arc diagrams of RNA secondary structures.



http://www.e-rna.org/r-chie/

The offline version of R-chie, which requires first installing R4RNA is available here, or clone our git repository here How to install it:

- Ensure R is installed already, or download it freely from http://www.r-project.org/
- Download the R4RNA (https://github.com/jujubix/r-chie), open R and install the package:

```
install.packages("<path_to_file>/R4RNA", repos = NULL, type="source")
# Install the optparse and RColorBrewer
install.packages('optparse')
install.packages('RColorBrewer')
```

- Go to rna_tools/rna_tools_config_local.py and set RCHIE_PATH to the folder with RChie, e.g. `"/home/magnus/work/opt/r-chie/"`.

To test if Rchie works on your machine (from rna_align folder):

```
<path to your rchie>/rchie.R --msafile test_data/rchie_test_files/fasta.txt test_
↪data/rchie_test_files/helix.txt
```

you should have rchie.png file in the folder.

More at http://www.e-rna.org/r-chie/download.cgi

Cite: Daniel Lai, Jeff R. Proctor, Jing Yun A. Zhu, and Irmtraud M. Meyer (2012) R-chie: a web server and R package for visualizing RNA secondary structures. Nucleic Acids Research, first published online March 19, 2012. doi:10.1093/nar/gks241

plot_cov(*seqs*, *ss_cons*, *plot_fn='rchie.png'*, *verbose=False*)

Plot an RChie plot_conv.

Parameters

- **seqs** – seqs in the fasta format

- **ss_cons** – a string of secondary structure consensus, use only ().. Works with pseuoknots.

show()

write(*outfn*)

4.4.6 Renumber a pdb file according to alignment

4.4.6.1 renum_to_aln.py

renum_pdb_to_aln.py - renumber a pdb file based on the alignment.

author: A. Zyla under supervision of mmagnus

Warning: works only for single chain! and requires Biopython (tested with v1.68)

```
usage: renum_to_aln.py [-h] [-v] [--residue_index_start RESIDUE_INDEX_START]
                       [--outfn OUTFN]
                       seqid alignfn pdbfn
```

seqid
seq id in the alignemnt

alignfn
alignemnt in the Fasta format

pdbfn
pdb file

-h, --help
show this help message and exit

-v, --verbose
increase output verbosity

--residue_index_start <residue_index_start>
renumber starting number (default: 1)

--outfn <outfn>
output pdb file (default: pdbfn .pdb -> _out.pdb)

renum_pdb_to_aln.py - renumber a pdb file based on the alignment.

author: A. Zyla under supervision of mmagnus

Warning: works only for single chain! and requires Biopython (tested with v1.68)

rna_tools.tools.renum_pdb_to_aln.renum_pdb_to_aln.**get_parser**()

rna_tools.tools.renum_pdb_to_aln.renum_pdb_to_aln.**get_seq**(*alignfn*, *seqid*)

Get seq from an alignment with gaps.

Parameters

- **alignfn** (*str*) – a path to an alignment
- **seqid** (*str*) – seq id in an alignment

Usage:

```
>>> get_seq('test_data/ALN_OBJ1_OBJ2.fa', 'obj1')
SeqRecord(seq=SeqRecord(seq=Seq('GUUCAG------------------UGAC-',␣
↪SingleLetterAlphabet()), id='obj1', name='obj1', description='obj1', dbxrefs=[]),␣
↪id='<unknown id>', name='<unknown name>', description='<unknown description>',␣
↪dbxrefs=[])
```

Returns
SeqRecord

rna_tools.tools.renum_pdb_to_aln.renum_pdb_to_aln.**open_pdb**(*pdbfn*)

Open pdb with Biopython.

Parameters
pdbfn (*str*) – a path to a pdb structure

Returns
with a pdb structure

Return type
PDB Biopython object

rna_tools.tools.renum_pdb_to_aln.renum_pdb_to_aln.**renumber**(*seq_with_gaps*, *struc*, *residue_index_start*)

Renumber a pdb file.

Parameters

- **seq_with_gaps** (*str*) – a target sequence extracted from the alignment
- **struc** (*pdb*) – a structure
- **residue_index_start** (*int*) – starting number

Returns
BioPython Structure object

rna_tools.tools.renum_pdb_to_aln.renum_pdb_to_aln.**write_struc**(*struc*, *outfn*)

Write renumbered pdb with Biopython.

Parameters

- **struc** (*pdb*) – a renumbered structure
- **outfn** (*str*) – a path to a new, renumbered pdb file

Returns
writes to a file

Return type
none

4.5 Root Mean Square Deviation (RMSD)

4.5.1 rna_calc_rmsd

4.5.1.1 rna_calc_rmsd

rna_calc_rmsd.py - calculate RMSDs of structures to the target

If you still have problem with various number of atoms, check out this issue: get_rnapuzzle_ready: how to deal with `Alternate location indicator (https://github.com/mmagnus/rna-pdb-tools/issues/30).

The program is using (https://github.com/charnley/rmsd).

Example #1:

```
$ rna_calc_rmsd.py -t 6_0_solution_4GXY_rpr.pdb --model-selection=A:1-17+24-110+115-168␣
↪*.pdb
rmsd_calc_rmsd_to_target
--------------------------------------------------------------------------------
method: all-atom-built-in
# of models: 35
6_0_solution_4GXY_rpr.pdb 0.0 3409
6_Blanchet_1_rpr.pdb 22.31 3409
6_Blanchet_2_rpr.pdb 21.76 3409
6_Blanchet_3_rpr.pdb 21.32 3409
6_Blanchet_4_rpr.pdb 22.22 3409
6_Blanchet_5_rpr.pdb 24.17 3409
6_Blanchet_6_rpr.pdb 23.28 3409
6_Blanchet_7_rpr.pdb 22.26 3409
6_Bujnicki_1_rpr.pdb 36.95 3409
6_Bujnicki_2_rpr.pdb 30.9 3409
6_Bujnicki_3_rpr.pdb 32.1 3409
6_Bujnicki_4_rpr.pdb 32.04 3409
...
```

Example #2:

```
time rmsd_calc_to_target.py
  -t 5k7c_clean_onechain_renumber_as_puzzle_srr.pdb
  --target-selection A:1-48+52-63
  --model-selection A:1-48+52-63
  --target-ignore-selection A/57/O2\'
  clusters/*_AA.pdb

rmsd_calc_rmsd_to_target
--------------------------------------------------------------------------------
  target_selection:  A:1-48+52-63
  model_selection:   A:1-48+52-63
  target_ignore_selection:  A/57/O2'
  model_ignore_selection:
# of models: 801
fn,rmsd_all
pistol_thrs0.50A_clust01-000001_AA.pdb,7.596
pistol_thrs0.50A_clust02-000001_AA.pdb,7.766
```

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```
pistol_thrs0.50A_clust03-000001_AA.pdb,18.171
[..]
pistol_thrs0.50A_clust799-000001_AA.pdb,5.356
pistol_thrs0.50A_clust800-000001_AA.pdb,15.282
pistol_thrs0.50A_clust801-000001_AA.pdb,16.339
# of atoms used: 1237
csv was created!  rmsds.csv
rmsd_calc_to_target.py -t 5k7c_clean_onechain_renumber_as_puzzle_srr.pdb
37.93s user 1.07s system 87% cpu 44.650 total
```

Works also for multiple chains:

rna_calc_rmsd.py –model-selection='A:52+53+59+60+61+80+B:21+22+23' –target-selection='A:52+53+59+60+61+80+B:21+22+23' -t yC_5LJ3_U2U6_core_mdrFx_onlyTriplex_rpr.pdb yC_5LJ3_U2U6_core_mdrFx_addh_MD_1_rpr_rchain.pdb

```
usage: rna_calc_rmsd [-h] -t TARGET_FN [--ignore-files IGNORE_FILES]
                     [--target-selection TARGET_SELECTION]
                     [--target-ignore-selection TARGET_IGNORE_SELECTION]
                     [--model-selection MODEL_SELECTION]
                     [--model-ignore-selection MODEL_IGNORE_SELECTION]
                     [-m METHOD] [-o RMSDS_FN] [-v] [-pr] [-sr] [-pp]
                     [--way WAY] [--name-rmsd-column NAME_RMSD_COLUMN]
                     [--target-column-name]
                     files [files ...]
```

files

files

-h, --help

show this help message and exit

-t <target_fn>, **--target-fn** <target_fn>

pdb file

--ignore-files <ignore_files>

files to be ingored, .e.g, 'solution'

--target-selection <target_selection>

selection, e.g. A:10-16+20, where #16 residue is included

--target-ignore-selection <target_ignore_selection>

A/10/O2'

--model-selection <model_selection>

selection, e.g. A:10-16+20, where #16 residue is included

--model-ignore-selection <model_ignore_selection>

A/10/O2'

-m <method>, **--method** <method>

align, fit

-o <rmsds_fn>, **--rmsds-fn** <rmsds_fn>

ouput, matrix

-v, --verbose

verbose

-pr, --print-results

-sr, --sort-results

-pp, --print-progress

--way <way>

R|c1p = C1' backbone = P OP1 OP2 O5' C5' C4' C3' O3' po = P OP1 OP2 no-backbone = all - po bases, backbone+sugar, sugar pooo = P OP1 OP2 O5' alpha = P OP1 OP2 O5' C5'

--name-rmsd-column <name_rmsd_column>

default: fn,rmsd, with this cols will be fn,<name-rmsd-column>

--target-column-name

rna_calc_rmsd.py - calculate RMSDs of structures to the target

If you still have problem with various number of atoms, check out this issue: get_rnapuzzle_ready: how to deal with `Alternate location indicator (https://github.com/mmagnus/rna-pdb-tools/issues/30).

The program is using (https://github.com/charnley/rmsd).

Example #1:

```
$ rna_calc_rmsd.py -t 6_0_solution_4GXY_rpr.pdb --model-selection=A:1-17+24-110+115-168␣
↪*.pdb
rmsd_calc_rmsd_to_target
--------------------------------------------------------------------------------
method: all-atom-built-in
# of models: 35
6_0_solution_4GXY_rpr.pdb 0.0 3409
6_Blanchet_1_rpr.pdb 22.31 3409
6_Blanchet_2_rpr.pdb 21.76 3409
6_Blanchet_3_rpr.pdb 21.32 3409
6_Blanchet_4_rpr.pdb 22.22 3409
6_Blanchet_5_rpr.pdb 24.17 3409
6_Blanchet_6_rpr.pdb 23.28 3409
6_Blanchet_7_rpr.pdb 22.26 3409
6_Bujnicki_1_rpr.pdb 36.95 3409
6_Bujnicki_2_rpr.pdb 30.9 3409
6_Bujnicki_3_rpr.pdb 32.1 3409
6_Bujnicki_4_rpr.pdb 32.04 3409
...
```

Example #2:

```
time rmsd_calc_to_target.py
  -t 5k7c_clean_onechain_renumber_as_puzzle_srr.pdb
  --target-selection A:1-48+52-63
  --model-selection A:1-48+52-63
  --target-ignore-selection A/57/O2\'
  clusters/*_AA.pdb

rmsd_calc_rmsd_to_target
```

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```
--------------------------------------------------------------------------------
  target_selection:  A:1-48+52-63
  model_selection:   A:1-48+52-63
  target_ignore_selection:  A/57/O2'
  model_ignore_selection:
# of models: 801
fn,rmsd_all
pistol_thrs0.50A_clust01-000001_AA.pdb,7.596
pistol_thrs0.50A_clust02-000001_AA.pdb,7.766
pistol_thrs0.50A_clust03-000001_AA.pdb,18.171
[..]
pistol_thrs0.50A_clust799-000001_AA.pdb,5.356
pistol_thrs0.50A_clust800-000001_AA.pdb,15.282
pistol_thrs0.50A_clust801-000001_AA.pdb,16.339
# of atoms used: 1237
csv was created!  rmsds.csv
rmsd_calc_to_target.py -t 5k7c_clean_onechain_renumber_as_puzzle_srr.pdb
37.93s user 1.07s system 87% cpu 44.650 total
```

Works also for multiple chains:

> rna_calc_rmsd.py –model-selection='A:52+53+59+60+61+80+B:21+22+23' –target-selection='A:52+53+59+60+61+80+B:21+22+23' -t yC_5LJ3_U2U6_core_mdrFx_onlyTriplex_rpr.pdb yC_5LJ3_U2U6_core_mdrFx_addh_MD_1_rpr_rchain.pdb

rna_tools.tools.rna_calc_rmsd.rna_calc_rmsd.**calc_rmsd**(*a*, *b*, *target_selection*, *target_ignore_selection*, *model_selection*, *model_ignore_selection*, *way*, *verbose*)

> Calculate RMSD between two XYZ files
>
> by: Jimmy Charnley Kromann <jimmy@charnley.dk> and Lars Andersen Bratholm <larsbratholm@gmail.com> project: https://github.com/charnley/rmsd license: https://github.com/charnley/rmsd/blob/master/LICENSE
>
> a is model b is target
>
> **Params**
> a = filename of structure a
>
> **Params**
> b = filename of structure b
>
> **Returns**
> rmsd, number of atoms

rna_tools.tools.rna_calc_rmsd.rna_calc_rmsd.**calc_rmsd_pymol**(*pdb1*, *pdb2*, *method*)

> Calculate rmsd using PyMOL. Two methods are available: align and fit
>
> See:
>
> - Align: <http://www.pymolwiki.org/index.php/Align>
> - Fit: <http://www.pymolwiki.org/index.php/Fit>
>
> Align can return a list with 7 items:
>
> - RMSD after refinement
> - Number of aligned atoms after refinement
> - Number of refinement cycles

- RMSD before refinement
- Number of aligned atoms before refinement
- Raw alignment score
- Number of residues aligned

in this version of function, the function returns *RMSD before refinement*.

Install on OSX: `brew install brewsci/bio/pymol` or get

If you have a problem:

```
Match-Error: unable to open matrix file '/opt/local/Library/Frameworks/Python.
↪framework/Versions/2.7/lib/python2.7/site-packages/data/pymol/matrices/BLOSUM62'.
```

then find BLOSUM62, e.g.:

```
mdfind -name BLOSUM62 | grep pymol
/Users/magnus/miniconda2/envs/py37/lib/python3.7/site-packages/pymol/pymol_path/
↪data/pymol/matrices/BLOSUM62
/usr/local/Cellar/pymol/2.4.0_3/libexec/lib/python3.9/site-packages/pymol/pymol_
↪path/data/pymol/matrices/BLOSUM62
/Users/magnus/miniconda2/pkgs/pymol-2.4.2-py37h06d7bae_0/share/pymol/data/pymol/
↪matrices/BLOSUM62
/Users/magnus/work/opt/pymol-open-source/data/pymol/matrices/BLOSUM62
```

and then define `PYMOL_DATA` in your .bashrc/.zshrc, e.g.:

```
export PYMOL_DATA="/Users/magnus/work/opt/pymol-open-source/data/pymol"
```

rna_tools.tools.rna_calc_rmsd.rna_calc_rmsd.**get_parser**()

rna_tools.tools.rna_calc_rmsd.rna_calc_rmsd.**get_rna_models_from_dir**(*files*)

Parameters
models – a list of filenames

Example of the list:

```
['test_data/rp17/2_restr1_Michal1.pdb_clean.pdb', 'test_data/rp17/2a_nonrestr2_
↪Michal1.pdb_clean.pdb',
'test_data/rp17/3_nonrestr1_Michal1.pdb_clean.pdb', 'test_data/rp17/5_restr1_
↪Michal3.pdb_clean.pdb']
```

rna_tools.tools.rna_calc_rmsd.rna_calc_rmsd.**sort_nicely**(*l*)

Sort the given list in the way that humans expect.

http://blog.codinghorror.com/sorting-for-humans-natural-sort-order/

4.5.1.2 rna_calc_rmsd_multi_targets.py

rna_calc_rmsd_multi_targets.py - calculate RMSDs of structures to multiple targets:

```
$ rna_calc_rmsd_multi_targets.py --models multi-targets/rp21/*.pdb
↪              --targets multi-targets/rp21/solutions/*.pdb
↪        --target-selection A:1-27+29-41                                --model-
↪selection A:1-27+29-41
```

CSV table produced:

```
                        21_solution_0_ChainA.pdb  21_solution_0_ChainB.pdb  21_
↪solution_1_ChainA.pdb  21_solution_1_ChainB.pdb  21_solution_2.pdb   mean    min
↪max    sd
fn
21_3dRNA_1_rpr.pdb                          12.17                      12.11
↪        12.17                     12.11             12.11  12.13  12.11  12.17  0.03
21_Adamiak_1_rpr.pdb                         4.64                       4.61
↪         4.64                      4.61              4.64   4.63   4.61   4.64  0.01
21_ChenHighLig_1_rpr.pdb                     4.01                       3.97
↪         4.01                      3.97              4.07   4.01   3.97   4.07  0.04
21_Das_1_rpr.pdb                             5.71                       5.60
↪         5.71                      5.60              5.61   5.65   5.60   5.71  0.05
--------------------------------------------------------------------------------
Save rna_calc_rmsd_multi_targets_output.csv
```

```
usage: rna_calc_rmsd_multi_targets.py [-h] [-v] [--models MODELS [MODELS ...]]
                                      [--targets TARGETS [TARGETS ...]]
                                      [--output-csv OUTPUT_CSV]
                                      [--model-selection MODEL_SELECTION]
                                      [--target-selection TARGET_SELECTION]
```

-h, --help
: show this help message and exit

-v, --verbose
: be verbose

--models <models>

--targets <targets>

--output-csv <output_csv>

--model-selection <model_selection>
: selection, e.g. A:10-16+20, where #16 residue is included

--target-selection <target_selection>
: selection, e.g. A:10-16+20, where #16 residue is included

4.5.2 rna_calc_rmsd_trafl

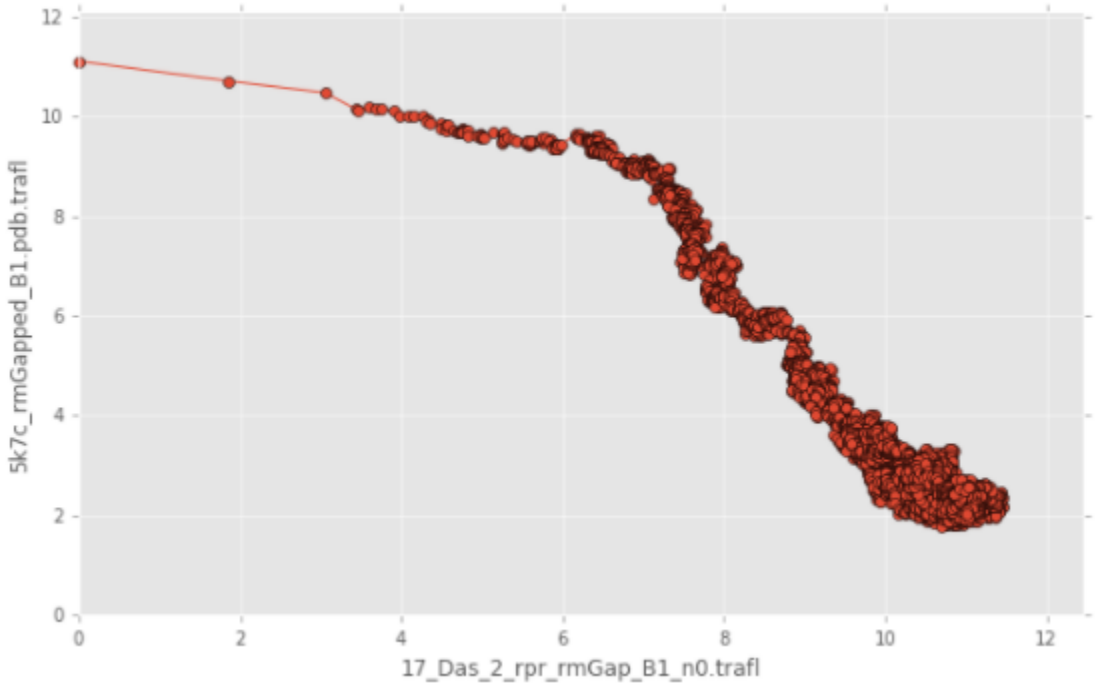
4.5.2.1 rna_calc_evo_rmsd

rmsd_calc_trafl - calculate RMSD of transition A->B based on a SimRNA trajectory

After this script, run:

```
rna_cal_rmsd_trafl_plot.py rmsd.txt
```

to get a plot like this:



Prepare structures:

```
$ SimRNA -p 17_Das_2_rpr.pdb -n 0 -o 17_Das_2_rpr_n0 # no trafl, trafl will be added
$ SimRNA -p 5k7c_clean_onechain_renumber_as_puzzle_rpr_rmGapped.pdb -n 0 -o 5k7c_clean_
↪onechain_renumber_as_puzzle_rpr_rmGapped
#(struc must be (~CG~) nope. It has to be a trajectory!)
```

and run:

```
 $ rmsd_calc_trafl.py 17_Das_2_rpr.pdb.trafl 17_Das_2_rpr_n0.trafl 5k7c_clean_onechain_
↪renumber_as_puzzle_rpr_rmGapped_n0.trafl rp17_rmsd.txt
 > calc_rmsd_to_1st_frame
   /Users/magnus/work/opt/simrna/SimRNA_64bitIntel_MacOSX_staticLibs/calc_rmsd_to_1st_
↪frame 17_Das_2_rpr.pdb.trafl 17_Das_2_rpr.pdb_rmsd_e
 < rmsd_out: 17_Das_2_rpr.pdb_rmsd_e
 > struc: 17_Das_2_rpr_n0.trafl 2
 > trafl: 17_Das_2_rpr.pdb.trafl 48
 % saved: 17_Das_2_rpr.pdb.trafl_17_Das_2_rpr_n0.trafl
 > calc_rmsd_to_1st_frame
```

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```
   /Users/magnus/work/opt/simrna/SimRNA_64bitIntel_MacOSX_staticLibs/calc_rmsd_to_1st_
↪frame 17_Das_2_rpr.pdb.trafl_17_Das_2_rpr_n0.trafl 17_Das_2_rpr.pdb_rmsd_e_17_Das_2_
↪rpr_n0_rmsd_e
 < rmsd_out: 17_Das_2_rpr.pdb_rmsd_e_17_Das_2_rpr_n0_rmsd_e
 > struc: 5k7c_clean_onechain_renumber_as_puzzle_rpr_rmGapped_n0.trafl 2
 > trafl: 17_Das_2_rpr.pdb.trafl 48
 % saved: 17_Das_2_rpr.pdb.trafl_5k7c_clean_onechain_renumber_as_puzzle_rpr_rmGapped_n0.
↪trafl
 > calc_rmsd_to_1st_frame
   /Users/magnus/work/opt/simrna/SimRNA_64bitIntel_MacOSX_staticLibs/calc_rmsd_to_1st_
↪frame 17_Das_2_rpr.pdb.trafl_5k7c_clean_onechain_renumber_as_puzzle_rpr_rmGapped_n0.
↪trafl 17_Das_2_rpr.pdb_rmsd_e_5k7c_clean_onechain_renumber_as_puzzle_rpr_rmGapped_n0_
↪rmsd_e
 < rmsd_out: 17_Das_2_rpr.pdb_rmsd_e_5k7c_clean_onechain_renumber_as_puzzle_rpr_rmGapped_
↪n0_rmsd_e
  0.000 -695.634
  0.000 -551.093
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
 < out: rp17_rmsd.txt
```

Warning: calc_rmsd_to_1st_frame (SimRNA) is required and the path to the binary file is defined in `config_local`.

```
usage: rna_calc_evo_rmsd [-h] trafl struc1 struc2 rmsds_fn
```

trafl
: trafil

struc1
: structure A

struc2
: structure B

rmsds_fn
: output file

-h, --help
: show this help message and exit

4.5.2.2 rna_cal_rmsd_trafl_plot

rna_cal_rmsd_trafl_plot - generate a plot based of <rmsd.txt> of rna_calc_evo_rmsd.py.

```
usage: rna_cal_rmsd_trafl_plot [-h] file
```

file
: rmsd.txt

-h, --help
: show this help message and exit

4.5.3 rna_calc_rmsd_all_vs_all

4.5.3.1 rna_calc_rmsd_all_vs_all

rna_calc_rmsd_all_vs_all.py - calculate RMSDs all vs all and save it to a matrix

Examples:

```
rna_calc_rmsd_all_vs_all.py -i test_data -o test_output/rmsd_calc_dir.tsv
 # of models: 4
... 1 test_data/struc1.pdb
... 2 test_data/struc2.pdb
... 3 test_data/struc3.pdb
... 4 test_data/struc4.pdb
```

The program is using (https://github.com/charnley/rmsd).

You can also use PyMOL to do align or fit:

```
python rna_calc_rmsd_all_vs_all.py -i test_data -o test_output/rmsd_calc_dir_align.mat -
↪m align
 # of models: 5
# test_data/2nd_triplex_FB_1AUA3_rpr.pdb test_data/struc1.pdb test_data/struc2.pdb test_
↪data/struc3.pdb test_data/struc4.pdb
0.0 4.13 4.922 4.358 4.368
4.13 0.0 11.092 4.707 3.46
4.922 11.092 0.0 11.609 11.785
4.358 4.707 11.609 0.0 2.759
4.368 3.46 11.785 2.759 0.0
matrix was created!  test
```

```
usage: rna_calc_rmsd_all_vs_all [-h] [-i INPUT_DIR] [-o MATRIX_FN] [-m METHOD]
```

-h, **--help**
: show this help message and exit

-i <input_dir>, **--input-dir** <input_dir>
: input folder with structures

-o <matrix_fn>, **--matrix-fn** <matrix_fn>
: ouput, matrix

-m <method>, **--method** <method>
: all-atom, pymol: align, fit

rna_calc_rmsd_all_vs_all.py - calculate RMSDs all vs all and save it to a matrix

Examples:

```
rna_calc_rmsd_all_vs_all.py -i test_data -o test_output/rmsd_calc_dir.tsv
 # of models: 4
... 1 test_data/struc1.pdb
... 2 test_data/struc2.pdb
... 3 test_data/struc3.pdb
... 4 test_data/struc4.pdb
```

The program is using (https://github.com/charnley/rmsd).

You can also use PyMOL to do align or fit:

```
python rna_calc_rmsd_all_vs_all.py -i test_data -o test_output/rmsd_calc_dir_align.mat -
↪m align
 # of models: 5
# test_data/2nd_triplex_FB_1AUA3_rpr.pdb test_data/struc1.pdb test_data/struc2.pdb test_
↪data/struc3.pdb test_data/struc4.pdb
0.0 4.13 4.922 4.358 4.368
4.13 0.0 11.092 4.707 3.46
4.922 11.092 0.0 11.609 11.785
4.358 4.707 11.609 0.0 2.759
4.368 3.46 11.785 2.759 0.0
matrix was created!  test
```

rna_tools.tools.rna_calc_rmsd.rna_calc_rmsd_all_vs_all.**calc_rmsd**(*a*, *b*)

Calc rmsd.

rna_tools.tools.rna_calc_rmsd.rna_calc_rmsd_all_vs_all.**get_parser**()

rna_tools.tools.rna_calc_rmsd.rna_calc_rmsd_all_vs_all.**get_rna_models_from_dir**(*directory*)

rna_tools.tools.rna_calc_rmsd.rna_calc_rmsd_all_vs_all.**sort_nicely**(*l*)

Sort the given list in the way that humans expect. http://blog.codinghorror.com/sorting-for-humans-natural-sort-order/

4.6 Interaction Network Fidelity (INF)

4.6.1 rna_calc_inf.py

```
usage: rna_calc_inf.py [-h] [-t TARGET_FN] [-m NT]
                       [--ignore-files IGNORE_FILES] [-s SS] [--no-stacking]
                       [--debug] [--web] [-pr] [-sr] [--method METHOD]
                       [--target-selection TARGET_SELECTION]
                       [--model-selection MODEL_SELECTION]
                       [--renumber-residues] [--dont-remove-sel-files] [-f]
                       [-v] [-o OUT_FN]
                       files [files ...]
```

files

files, .e.g folder_with_pdbs/*pdbs

-h, **--help**

show this help message and exit

-t <target_fn>, **--target_fn** <target_fn>

pdb file

-m <nt>, **--number-of-threads** <nt>

number of threads used for multiprocessing, if 1 then mp is not used (useful for debugging)!

--ignore-files <ignore_files>
files to be ingored, .e.g, 'solution'

-s <ss>, **--ss** <ss>
A:(([[]))]], works only for single chain (the chain is A by default)

--no-stacking
default: use stacking, if this option on, don't take into account stacking,

WARNING/BUG: inf_all will be incorrectly calculated if stacking is off

--debug

--web

-pr, **--print-results**

-sr, **--sort-results**

--method <method>
you can use mcannotate* or clarna (right now only clarna is tested)

--target-selection <target_selection>
selection, e.g. A:10-16+20, where #16 residue is included

--model-selection <model_selection>
selection, e.g. A:10-16+20, where #16 residue is included

--renumber-residues
renumber residues from 1 to X for comparison with selection

--dont-remove-sel-files
don't remove temp files created based on target|model-selectionforce

-f, **--force**
force to run ClaRNA even if <pdb>.outCR file is there, for will be auto True when selection defined

-v, **--verbose**
be verbose, tell me more what're doing

-o <out_fn>, **--out_fn** <out_fn>
out csv file, be default *inf.csv*

A tool to calc inf_all, inf_stack, inf_WC, inf_nWC, SNS_WC, PPV_WC, SNS_nWC, PPV_nWC between two structures.

Mind, that ClaRNA is pretty slow, it takes even a few seconds to analyze a structure, so for, say, 1000 models you need a few hours.

How to make it faster?

First, you can use `--number-of-threads` to specify the number of cores used for multiprocessing.

Second, the procedure implemented in here is composed of two steps, first for each structure ClaRNA is used to generate an output with contacts, then these files are used for comparisons. So, if you want to re-run your analysis, you don't have to re-run ClaRNA itself. Thus, be default ClaRNA is not executed if <model>.outCR is found next to the analyzed files. To change this behavior, force (`--force`) rna_calc_inf.py to re-run ClaRNA.

rna_tools.tools.rna_calc_inf.rna_calc_inf.**do_job**(*l*)
Run ClaRNA & Compare, add 1 to the counter, write output to csv file (keeping it locked)

rna_tools.tools.rna_calc_inf.rna_calc_inf.**get_parser**()

4.7 RNA filter (DCA)

4.7.1 Calculate distances based on given restrants on PDB files or SimRNA trajectories

4.7.1.1 rna_filter.py

rna_filter.py - calculate distances based on given restrants on PDB files or SimRNA trajectories.

Changes: weight is always 1 (at least for now). ,>,=,>=,<= .

[PREVIOUS DOCUMENTATION - TO BE REMOVED]

rna_filter.py -s 4gxy_rpr.pdb -r rp06_MohPairs.rfrestrs d:A5-A42 100.0 measured: 26.7465763417 [x] d:A11-A26 100.0 measured: 19.2863696104 [x]

[mm] rp06$ git:(master) $ rna_filter.py -s 4gxy_rpr.pdb -r rp06_MohPairs.rfrestrs
d:A5-A42 100.0 measured: 26.7465763417 [x] d:A11-A26 100.0 measured: 19.2863696104 [x]

Traceback (most recent call last):

File "/home/magnus/work-src/rna-pdb-tools/bin/rna_filter.py", line 270, in <module>
calc_scores_for_pdbs(args.structures, restraints, args.verbose)

File "/home/magnus/work-src/rna-pdb-tools/bin/rna_filter.py", line 221, in calc_scores_for_pdbs
dist = get_distance(residues[h[0]]['mb'], residues[h[1]]['mb'])

KeyError: 'A24'

correct, there is no A24 in this structure:

The format of restraints:

```
(d:A1-A2 < 10.0 1) = if distance between A1 and A2 lower than 10.0, score it with 1
```

Usage:

```
$ python rna_filter.py -r test_data/restraints.txt -s test_data/CG.pdb
 d:A1-A2 10.0 measured: 6.58677550096 [x]
test_data/CG.pdb 1.0 1 out of 1

# $ python rna_filter.py -r test_data/restraints.txt -t test_data/CG.trafl
(d:A1-A2 <  10.0  1)|(d:A2-A1 <= 10 1)
 restraints [('A1', 'A2', '<', '10.0', '1'), ('A2', 'A1', '<=', '10', '1')]

Frame #1 e:1252.26
  mb for A1 [ 54.729   28.9375  41.421 ]
  mb for A2 [ 55.3425  35.3605  42.7455]
   d:A1-A2 6.58677550096
  mb for A2 [ 55.3425  35.3605  42.7455]
  mb for A1 [ 54.729   28.9375  41.421 ]
   d:A2-A1 6.58677550096
# this ^ is off right now
```

```
usage: rna_filter.py [-h] -r RESTRAINTS_FN [-v]
                     [-s STRUCTURES [STRUCTURES ...]] [--offset OFFSET]
                     [-t TRAJECTORY]
```

-h, --help
show this help message and exit

-r <restraints_fn>, **--restraints_fn** <restraints_fn>
restraints_fn: Format: (d:A9-A41 < 10.0 1)|(d:A41-A9 <= 10 1)

-v, --verbose
be verbose

-s <structures>
structures

--offset <offset>
use offset to adjust your restraints to numbering in PDB files, ade (1y26)pdb starts with 13, so offset is -12)

-t <trajectory>
SimRNA trajectory

4.7.1.2 rna_dca_mapping.py

```
usage: rna_dca_mapping.py [-h] --seq SEQ --gseq GSEQ --dca DCA
                          [--offset OFFSET] [--noss] [--mss] [--verbose]
                          [--noshort]
```

-h, --help
show this help message and exit

--seq <seq>
seq fn in Fasta format

--gseq <gseq>
gapped sequence and secondary structure (like in the alignment used for DCA) in Fasta format

--dca <dca>
file with parsed interactions

--offset <offset>
offset

--noss
filter out ss from plot

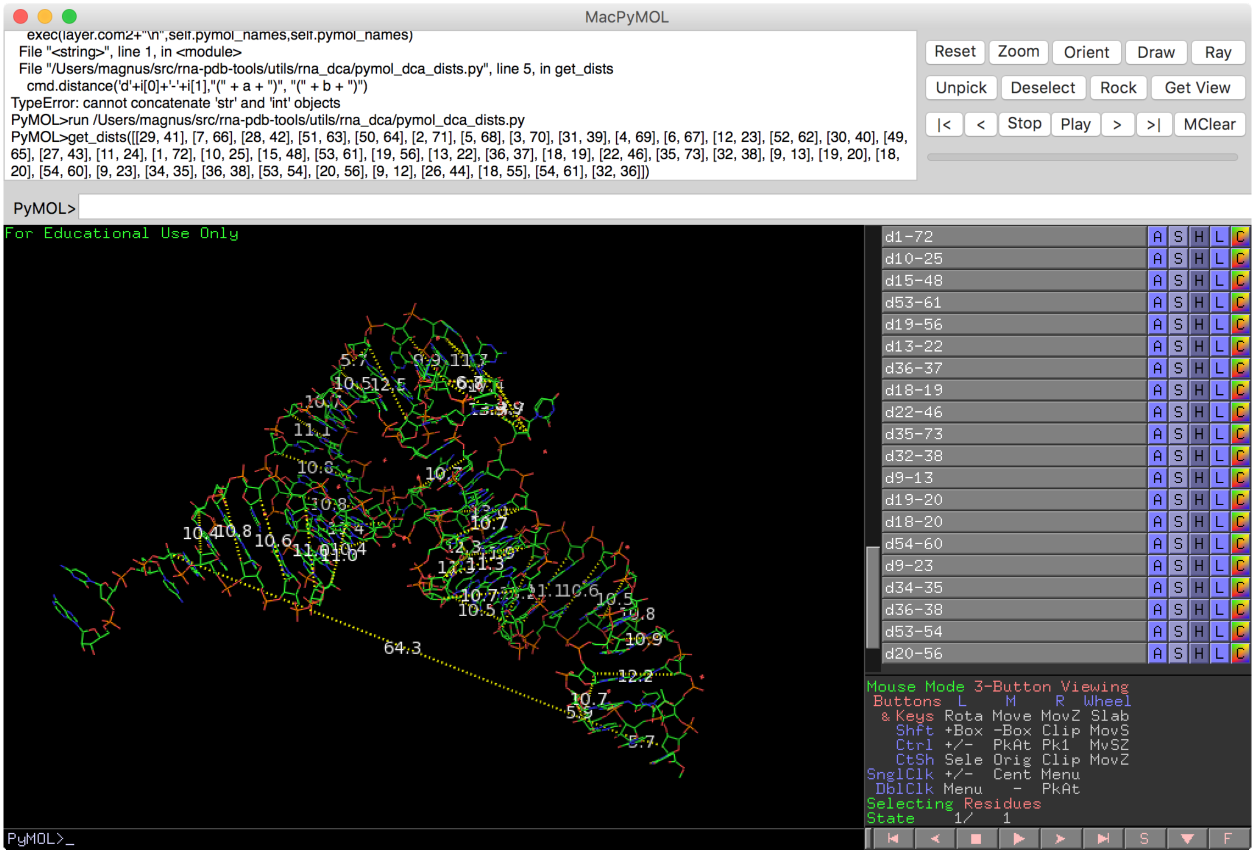
--mss
ss every each line

--verbose
be verbose

--noshort
filter out short interactions, dist in seq < 6 nt

4.7.2 Show distances in PyMOL

show_dists - show distances in PyMOL



Usage:

```
PyMOL>show_dists([[1,2]])
1, 2, 3.41
```

Analyze an evolutionary coupling file. ~~~~~~`

4.7.2.1 rna_ec2x.py

rna_ex2x.py - analyze an evolutionary coupling file.

Files can be downloaded from https://marks.hms.harvard.edu/ev_rna/, e.g. RF00167.EC.interaction.csv

`--pairs`:

```
$ rna_ex2x.py RF00167.EC.interaction_LbyN.csv --pairs
[18, 78],[31, 39],[21, 75],[30, 40],[28, 42],[27, 43],[59, 67],[54, 72],[57, 69],[25,
→45],[29, 41],[17, 79],[26, 44],[16, 80],[14, 82],[19, 77],[55, 71],[
   15, 81],[34, 63],[56, 70],[58, 68],[35, 63],[26, 45],[35, 64],[32, 39],[54, 73],[24,
→74],[16, 82],[24, 45],[24, 43],[32, 36],[25, 48],[48, 82],[36, 48],
```

```
usage: rna_ec2x.py [-h] [--sep SEP] [--chain CHAIN] [--ec-pairs]
                   [--ss-pairs SS_PAIRS] [--pairs-delta]
                   interaction_fn
```

interaction_fn
interaction file

-h, --help
show this help message and exit

--sep <sep>
separator

--chain <chain>
chain

--ec-pairs

--ss-pairs <ss_pairs>
file with secondary structure base pairs

--pairs-delta
delta: ec-bp - ss-paris

4.7.3 Convert pairs to SimRNA restraints

4.7.3.1 rna_pairs2SimRNArestrs.py

rna_pairs2SimRNArestrs.py - convert pairs to SimRNA restraints

Example:

```
$ rna_pairs2SimRNArestrs.py rp06_pairs_delta.txt -v
# of pairs: 42
SLOPE A/2/MB A/172/MB 0 6 1
SLOPE A/2/MB A/172/MB 0 7 -1
SLOPE A/3/MB A/169/MB 0 6 1
SLOPE A/3/MB A/169/MB 0 7 -1
SLOPE A/12/MB A/32/MB 0 6 1
```

```
usage: rna_pairs2SimRNArestrs.py [-h] [--offset OFFSET] [--weight WEIGHT]
                                 [--dist DIST] [--well] [-v]
                                 pairs
```

pairs
a file with [[2, 172], [3, 169], [12, 32], [13, 31]]

-h, --help
show this help message and exit

--offset <offset>
can be -10

--weight <weight>
weight

--dist <dist>
distances, for MOHCA use 25

--well
well instead of slope

-v, --verbose
be verbose

4.7.4 Get a list of base pairs for a given "fasta ss" file.

4.7.4.1 rna_ss_get_bps.py

rna_ss_get_bps.py - get a list of base pairs for a given "fasta ss" file.

Input file:

```
cat ade_ss.fa
>1y26
CGCUUCAUAUAAUCCUAAUGAUAUGGUUUGGGAGUUUCUACCAAGAGCCUUAAACUCUUGAUUAUGAAGUG
(((((((((...((((((.........))))))........((((((.......))))))..)))))))))%
```

Usage:

```
$ rna_ss_get_bps.py ade_ss.fa --offset 12
[[13, 83], [14, 82], [15, 81], [16, 80], [17, 79], [18, 78], [19, 77], [20, 76], [21,␣
↪75], [25, 45], [26, 44], [27, 43], [28, 42], [29, 41], [30, 40], [54, 72], [55, 71],␣
↪[56, 70], [57, 69], [58, 68], [59, 67]]
```

Now it also work with pseudoknots.

```
usage: rna_ss_get_bps.py [-h] [--offset OFFSET] [-v] file
```

file
file in the Fasta format

-h, --help
show this help message and exit

--offset <offset>
offset

-v, --verbose
be verbose

4.7.5 Get a diff of pairs

4.7.5.1 rna_pairs_diff.py

rna_pairs_diff.py - get a diff of pairs

Usage:

```
$ rna_pairs_diff.py pistol_dca_all.bp pistol.bp
# of ec_paris: 31
# of ssbps   : 18
dalta#       : 13
[[4, 32], [6, 9], [6, 36], [6, 39], [9, 39], [13, 32], [16, 17], [17, 18], [22, 49], [29,
↪ 58]]
```

```
usage: rna_pairs_diff.py [-h] [-v] pairs1 pairs2
```

pairs1
: a list of pairs, A

pairs2
: a list of pairs to subtract, A-B, results in C(all pairs that are in A and are not in B

-h, --help
: show this help message and exit

-v, --verbose
: be verbose

4.8 Contacts classification & secondary structure detection

See also PyMOL4RNA for ways to visualize edges https://rna-tools.readthedocs.io/en/latest/pymol4rna.html

4.8.1 3DNA (contacts classification & secondary structure detection)

Python parser to 3dna <http://x3dna.org/>.

Installation:

```
# install the code from http://forum.x3dna.org/downloads/3dna-download/
Create a copy of the rna_x3dna_config_local_sample.py (remove "_sample") present in rna-
↪tools/rna_tools/tools/rna_x3dna folder.
Edit this line :
BINARY_PATH = <path to your x3dna-dssr file>
matching the path with the path of your x3dna-dssr file.
e.g. in my case: BINARY_PATH = ~/bin/x3dna-dssr.bin
```

For one structure you can run this script as:

```
[mm] py3dna$ git:(master)  ./rna_x3dna.py test_data/1xjr.pdb
test_data/1xjr.pdb
>1xjr nts=47 [1xjr] -- secondary structure derived by DSSR
```

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```
gGAGUUCACCGAGGCCACGCGGAGUACGAUCGAGGGUACAGUGAAUU
..(((((((...((((.((((.....)).)).)).))).).)))))))
```

For multiple structures in the folder, run the script like this:

```
[mm] py3dna$ git:(master)  ./rna_x3dna.py test_data/*
test_data/1xjr.pdb
>1xjr nts=47 [1xjr] -- secondary structure derived by DSSR
gGAGUUCACCGAGGCCACGCGGAGUACGAUCGAGGGUACAGUGAAUU
..(((((((...((((.((((.....)).)).)).))).).)))))))
test_data/6TNA.pdb
>6TNA nts=76 [6TNA] -- secondary structure derived by DSSR
GCGGAUUUAgCUCAGuuGGGAGAGCgCCAGAcUgAAgAPcUGGAGgUCcUGUGtPCGaUCCACAGAAUUCGCACCA
(((((((..((((.....[..)))).((((.........)))).....(((((..].....)))))))))))....
test_data/rp2_bujnicki_1_rpr.pdb
>rp2_bujnicki_1_rpr nts=100 [rp2_bujnicki_1_rpr] -- secondary structure derived by DSSR
CCGGAGGAACUACUG&CCGGCAGCCU&CCGGAGGAACUACUG&CCGGCAGCCU&CCGGAGGAACUACUG&CCGGCAGCCU&
↪CCGGAGGAACUACUG&CCGGCAGCCU
[[[[[((.....(((&{{{{}))))))&(((((((.....(.(&]]]]).))))&[[[[[[.....[[[&)))))]]].]]&}}}}(((.
↪....(((&]]]]))))))
```

Warning: This script should not be used in this given form with Parallel because it process output files from x3dna that are named always in the same way, e.g. dssr-torsions.txt. #TODO

rna_tools.tools.rna_x3dna.rna_x3dna.**get_parser**()

class rna_tools.tools.rna_x3dna.rna_x3dna.**x3DNA**(*pdbfn*, *show_log=False*)

Atributes:

curr_fn report

clean_up(*verbose=False*)

get_ion_water_report()

@todo File name: /tmp/tmp0pdNHS

no. of DNA/RNA chains: 0 [] no. of nucleotides: 174 no. of waters: 793 no. of metals: 33 [Na=29, Mg=1, K=3]

get_modifications()

Run find_pair to find modifications.

get_secstruc()

Get secondary structure.

get_seq()

Get sequence.

Somehow 1bzt_1 x3dna UCAGACUUUUAAPCUGA, what is P? P -> u

get_torsions(*outfn*) → str

Get torsion angles into 'torsion.csv' file:

nt,id,res,alpha,beta,gamma,delta,epsilon,zeta,e-z,chi,phase-angle,sugar-type,ssZp,Dp,splay,bpseq
1,g,A.GTP1,nan,nan,142.1,89.5,-131.0,-78.3,-53(BI),-178.2(anti),358.6(C2'-exo),~C3'-endo,4.68,4.68,29.98,0 2,G,A.G2,-75.8,-167.0,57.2,79.5,-143.4,-69.7,-74(BI),-169.2(anti),5.8(C3'-endo),~C3'-endo,4.68,4.76,25.61,0

run_x3dna(*show_log=False*, *verbose=False*)

exception rna_tools.tools.rna_x3dna.rna_x3dna.**x3DNAMissingFile**

4.8.2 ClaRNA (contacts classification)

If you want to calculate "Interaction Network Fidelity (INF) and not only" see also rna_calc_inf

To run ClaRNA, see the documentaton below: Usage:

```
$ rna_clarna_app.py ../../input/5k7c_clean_onechain_renumber_as_puzzle_srr.pdb
↪  ../../input/5k7c_clean_onechain_renumber_as_puzzle_srr.pdb
((((((((((.))))).....(.((....(]]]]]].)..(((.....)))...)).)
```

Example

```
from rna_tools.utils.clarna_app import clarna_app
if __name__ == '__main__':
    ss = '((((.[[[[[[.))))........((((.....]]]]]]...(((((....)))))..))))'
    fnCRref = clarna_app.get_ClaRNA_output_from_dot_bracket(ss)
    f = '../rna_calc_rmsd/test_data/pistol/5k7c_clean_onechain_renumber_as_puzzle_srr.pdb
↪'
    fnCR = clarna_app.clarna_run(f, force=False)
    results = clarna_app.clarna_compare(fnCRref, fnCR)
    print results #
    #tmp_Z42i_..pdb.outCR     5k7c_clean_onechain_renumber_as_puzzle_srr.pdb.outCR
↪0.706      NA          0.865      NA          0.842      0.889      NA          0.000
```

rna_tools.tools.clarna_app.rna_clarna_app.**clarna_compare**(*target_cl_fn*, *i_cl_fn*, *verbose=False*)

Run ClaRNA compare (from rna_tools/tools/clarna_play).

Returns
a list target, fn, scores

Scores:

```
inf_all      0.706
inf_stack -999.999 -> NA
inf_WC       0.865
inf_nWC   -999.999 -> NA
SNS_WC       0.842
PPV_WC       0.889
SNS_nWC     NA
PPV_nWC      0.000
```

Example of the list:

```
5k7c_clean_onechain_renumber_as_puzzle_srr.pdb     pistol_thrs0.50A_clust01-000001_
↪AA.pdb
 0.642       NA          0.874       0.000       0.944       0.810       0.000       0.000s
```

use `results.split()[4]` to get inf_WC

rna_tools.tools.clarna_app.rna_clarna_app.**clarna_run**(*fn*, *force=True*, *stacking=True*, *verbose=False*)

Run ClaRNA run

Parameters
fn (*str*) – filename to analyze

Returns
a filename to ClaRNA output (fn + '.outCR')

Return type
str

rna_tools.tools.clarna_app.rna_clarna_app.**get_ClaRNA_output_from_dot_bracket**(*ss*, *temp=True*, *verbose=False*)

Get dummy ClaRNA output out of dat bracket secondary structure (ss)

Parameters
ss (*string*) – secondary structure

Returns
a filename to ClaRNA output

rna_tools.tools.clarna_app.rna_clarna_app.**get_dot_bracket_from_ClaRNAoutput**(*inCR*, *verbose=False*)

In inCR file

Warning: This function requres 'ClaRNAwd_to_vienaSS' contact marcin.magnus@icloud.com

rna_tools.tools.clarna_app.rna_clarna_app.**get_parser**()

4.9 RNA 3D model quality assessment

Wrappers behind the server, http://genesilico.pl/mqapRNA (in short, mq)

4.9.1 RASP

This module contains functions for computing RASP potential

class rna_tools.tools.mq.RASP.RASP.**RASP**(*job_id=None*)

Wrapper class for running RASP automatically.

colour_by_local_score(*path_to_pdb*, *potential_type='all'*)

executable = ['rasp_fd', 'rasp_profile_fd']

program_name = ['rasp_fd', 'rasp_profile_fd']

run(*path_to_pdb*, *global_energy_score=True*, *potentials=['c3', 'bb', 'bbr', 'all']*, *handler=True*, *verbose=False*)

Compute RASP potential for a single file

rasp_fd generates:

output_all.txt:

```
-9869.61   66447       -0.148534       0       0       0
```

rasp_profile_fd generates:

profile_all.txt:

```
C           1       R       -775.038
C           2       R       -1164.22
U           3       R       -2054.17
G           4       R       -1601.13
[..]
```

Input:

- path_to_pdb = path to PDB file
- potential_type = all, bbr or c3
- global_energy_score = True/False (See Output), default=True
- hander = True (if you use PYRO)/FALSE otherwise

Output:

- the output depends on global_enery_score value T/F You might get:

  -9869.61

  profile [('C', 1, 'R', -775.03800000000001), ('C', 2, 'R', -1164.22) ..

4.9.2 Dfire

This module contains functions for computing Dfire potential

Installation:

git clone https://github.com/tcgriffith/dfire_rna.git make # add DFIRE_RNA_HOME to .bashrc

class rna_tools.tools.mq.Dfire.Dfire.**Dfire**

Wrapper class for Dfire.

run(*path_to_pdb*, *verbose=False*)

Run program with previously set flags. This method should work if program wants some command some options and nothing more, otherwise you should override it.

rna_tools.tools.mq.Dfire.Dfire.**get_parser**()

rna_tools.tools.mq.Dfire.Dfire.**test**(*verbose*)

4.9.3 RNAkb

This module contains functions for computing RNAkb potential

It seems that this is impossible to run RNAkb in full atom mode. So this works only in 5 pt (5 points/atom per residue) mode.

https://gromacs.bioexcel.eu/t/fatal-error-an-input-file-contains-a-line-longer-than-4095-characters/1397/2

class rna_tools.tools.mq.RNAkb.RNAkb.**RNAkb**(*job_id=''*, *sandbox=False*)

Wrapper class for running RNAkb automatically.

executable = ['/usr/local/gromacs/bin/pdb2gmx', '/usr/local/gromacs/bin/make_ndx', '/usr/local/gromacs/bin/editconf', '/usr/local/gromacs/bin/grompp', '/usr/local/gromacs/bin/mdrun']

log_stdout_stderr()

run(*name*, *potential_type*, *verbose=False*)

Compute RNAkb potential for a single file

Parameters

- **path** (*str*) – name of a PDB file
- **potential_type** (*str*) – '5pt' for 5 point or 'aa' for all atom aa is off

Returns

a list of energies (strings) ['2.57116e+05', '1.62131e+03', '7.82459e+02', '3.00789e-01', '0.00000e+00', '0.00000e+00', '-2.51238e-03', '0.00000e+00', '2.59520e+05', '2.54174e-09', '2.59520e+05']

Warning: 'aa' does not work because of "a line longer than 4095 characters"

The function parses:

```
Statistics over 1 steps using 1 frames
Energies (kJ/mol)
Bond          Angle    Proper Dih.  Improper Dih.          LJ-14
2.44111e+05    1.76069e+03    8.12947e+02    1.82656e-01    0.00000e+00
Coulomb-14        LJ (SR)   Coulomb (SR)      Potential    Kinetic En.
0.00000e+00   -1.94624e-03    0.00000e+00    2.46685e+05    2.43227e-09
Total Energy    Temperature Pressure (bar)
2.46685e+05    6.67884e-10   -5.94232e+04
Total Virial

# ['Statistics', 'over', '1', 'steps', 'using', '1', 'frames', 'Energies', '(kJ/mol)',
'Bond', 'Angle', 'Proper', 'Dih.', 'Improper', 'Dih.', 'LJ-14', '2.44111e+05',
↪'1.76069e+03',
'8.12947e+02', '1.82656e-01', '0.00000e+00', 'Coulomb-14', 'LJ', '(SR)',
↪'Coulomb', '(SR)',
'Potential', 'Kinetic', 'En.', '0.00000e+00', '-1.94624e-03', '0.00000e+00', '2.
↪46685e+05',
'2.43227e-09', 'Total', 'Energy', 'Temperature', 'Pressure', '(bar)', '2.
↪46685e+05', '6.67884e-10',
'-5.94232e+04', 'Total', 'Virial']
```

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```
result[6] is really the RNAkb
```

4.9.3.1 rna_mq_rnakb.py

Standalone tool to run the RNAkb class in the terminal.

All atom mode does not really work, see the documentation of the RNAkb class.

```
usage: rna_mq_rnakb.py [-h] [-v] [-p POTENTIAL] file [file ...]
```

file
: a PDB file, one or more

-h, --help
: show this help message and exit

-v, --verbose
: be verbose

-p <potential>, **--potential** <potential>
: 5pt

4.9.4 QRNA

4.9.5 eSCORE

This module contains functions for computing eSCORE

Install:

```
pip install barnaba # tested with barnaba==0.1.7
```

Output:

```
$ baRNAba ESCORE --pdb ../test/1a9n.pdb --ff /Users/magnus/work/opt/barnaba/barnaba_
↪201128/test/data/1S72.pdb
# your output will be written to files with prefix outfile.ESCORE
# KDE computed. Bandwidth=  0.25  using 10655 base-pairs# Loaded sample ../test/1a9n.pdb

#     Frame       ESCORE
          0   4.1693e-01
```

The eSCORE could be also accessed via Python:

```
from barnaba import escore
Escore = escore.Escore([path_to_pdb])
(..)
# see example_12_escore.ipynb of barnaba package https://github.com/srnas/barnaba
```

It does not work on M1 mac (problem to compile mdtraj).

class rna_tools.tools.mq.eSCORE.eSCORE.**eSCORE**

Wrapper class for eSCORE

run(*path_to_pdb*, *verbose=False*)

Run program with previously set flags. This method should work if program wants some command some options and nothing more, otherwise you should override it.

rna_tools.tools.mq.eSCORE.eSCORE.**exe**(*cmd*)

rna_tools.tools.mq.eSCORE.eSCORE.**main**()

4.9.6 3dRNAscore

This module contains functions for computing 3dRNAscore

Install:

```
make # make clean if you don't have clean
```

At Mac there is a problem (201128, 211103):

```
(py37) [mx] example$ ../bin/3dRNAscore -s:1 score.in >score.txt
[1]    69818 segmentation fault  ../bin/3dRNAscore -s:1 score.in > score.txt
```

class rna_tools.tools.mq.RNAscore.RNAscore.**RNAscore**(*job_id=None*)

Wrapper class for running 3dRNAscore

program_name = '/bin/3dRNAscore'

run(*path_to_pdb*, *verbose=1*)

Run program with previously set flags. This method should work if program wants some command some options and nothing more, otherwise you should override it.

rna_tools.tools.mq.RNAscore.RNAscore.**main**()

4.9.7 RNA3DCNN

This module contains functions for computing RNA3DCNN potential

Output:

```
Trainable params: 4,282,801
Non-trainable params: 0
_________________________________________________________________
Scores for each nucleotide in /var/folders/yc/ssr9692s5fzf7k165grnhpk80000gp/T/
↪tmptg6jy2ud/query.pdb:
[[ 0.02462262]
 [ 0.03271335]
 [ 0.06199259]
 [ 0.02006263]
 [ 0.05937254]
 [ 0.12025979]
 [ 0.20201728]
 [ 0.24463326]
```

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```
 [ 0.43518737]
 [ 0.7260638 ]
 [ 0.6140108 ]
 [ 0.6588027 ]
 [ 0.7668936 ]
 [ 0.4776191 ]
 [ 0.39859247]
 [ 0.572009  ]
 [ 0.64892375]
 [ 0.11587611]
 [ 0.0560993 ]
 [ 0.05285829]
 [ 0.0167731 ]
 [ 0.01759553]
 [ 0.02143204]
 [-0.01818037]]
Total score for /var/folders/yc/ssr9692s5fzf7k165grnhpk80000gp/T/tmptg6jy2ud/query.pdb␣
↪is  6.3262305
```

If missing atoms:

```
Total params: 4,282,801
Trainable params: 4,282,801
Non-trainable params: 0
_________________________________________________________________
There is no atom O5' in residue 620A in chain  A in PDB /var/folders/yc/
↪ssr9692s5fzf7k165grnhpk80000gp/T/tmpx87uus6x/query.pdb.
There is no atom O5' in residue 635A in chain  B in PDB /var/folders/yc/
↪ssr9692s5fzf7k165grnhpk80000gp/T/tmpx87uus6x/query.pdb.
There is no atom O5' in residue 1750G in chain  C in PDB /var/folders/yc/
↪ssr9692s5fzf7k165grnhpk80000gp/T/tmpx87uus6x/query.pdb.
Scores for each nucleotide in /var/folders/yc/ssr9692s5fzf7k165grnhpk80000gp/T/
↪tmpx87uus6x/query.pdb:
[]
Total score for /var/folders/yc/ssr9692s5fzf7k165grnhpk80000gp/T/tmpx87uus6x/query.pdb␣
↪is  0.0
```

class rna_tools.tools.mq.RNA3DCNN.RNA3DCNN.**RNA3DCNN**

Wrapper class for RNA3DCNN.

max_seq_len = 100000

run(*path_to_pdb*, *verbose=False*)

Run program with previously set flags. This method should work if program wants some command some options and nothing more, otherwise you should override it.

rna_tools.tools.mq.RNA3DCNN.RNA3DCNN.**main**()

4.9.8 FARNA

Wrapper for ROSETTA software for structure prediction of small RNA sequences

class rna_tools.tools.mq.FARNA.FARNA.**FARNA**(*sequence='test'*, *seq_name='test'*, *job_id=None*)

Wrapper class for running ROSETTA scoring function automatically.

best_energy = ''

cleanup()

Run this method when you are done with this wrapper. It deletes sandbox, some of it's childrem may do some other cleanup here.

db_path = ''

executable = 'rna_minimize'

get_result()

Parse and get result from score file created during ROSETTA run

All results are kept in self.result, but only global score is returned

input_file = ''

input_fn = 'seq.fasta'

mqap(*pdb*)

Total weighted score:s+(?P<ROSETTA_SCORE>[-d.]+)

program_name = 'farna'

run(*pdb_file*, *hires*, *verbose=False*, *system=False*)

Compute FARNA potential for a single file

Parameters

- **file** (** pdb_file = path to pdb*) –
- **True/False** (** global_energy_score =*) –

Output:

- A list of energies, e.g:

```
['-21.721', '-0.899', '-20.961', '-84.498', '-16.574', '-180.939', '11.
↪549', '7.475', '-17.257', '-306.324', '0.0', '0.0', '17.503', '0.0']
```

??? or a dictionary of lists of local scores, eg:

```
{
'N_BS': [17.0, -0.70039, -0.720981, -0.685238, -0.734146, ... ],
'atom_pair_constraint': [0.0, -0.764688, -0.773833, ...],
...
}
```

sandbox()

Create a sandbox in temporary folder for running program.

src_bin = ''

4.9.9 ClashScore

class rna_tools.tools.mq.ClashScore.ClashScore.**ClashScore**

ClashScore: Wrapper class for running phenix.clashscore

cleanup()

run(*fn*, *verbose=False*)

Parameters

- **fn** (*string*) – path to a file
- **verbose** (*bool*) – be verbose

Returns

clashscore (float)

Example:

```
/Applications/phenix-1.18.2-3874/build/bin/phenix.clashscore test/1xjrA.pdb
Using electron cloud x-H distances and vdW radii

Adding H/D atoms with reduce...

Bad Clashes >= 0.4 Angstrom:
 A  17    A  N1   A  34    G  N1  :0.430
clashscore = 0.66
test/1xjrA.pdb
0.66
/Applications/phenix-1.18.2-3874/build/bin/phenix.clashscore test/1xjrA_M1.pdb
Using electron cloud x-H distances and vdW radii

Adding H/D atoms with reduce...

Bad Clashes >= 0.4 Angstrom:
 A  41    G  H2'  A  42    U  OP1 :0.738
 A  25    U  H6   A  25    U HO2' :0.659
 A  46    U  H2'  A  47    U  OP2 :0.656
 A  29    A H5''  A  30    U  O2' :0.623
 (...)

  A  24    G  O2'  A  26    A  C8  :0.410
 A  42    U  O2'  A  43    G  H8  :0.409
 A  43    G  H2'  A  44    A  O4' :0.408
 A  28    G  C8   A  28    G  O2' :0.403
clashscore = 15.45
test/1xjrA_M1.pdb
15.45

# so the output is
clashscore = 15.45
```

rna_tools.tools.mq.ClashScore.ClashScore.**test**()

4.9.10 AnalyzeGeometry

This module contains functions for computing AnalyzeGeomotery.

class rna_tools.tools.mq.AnalyzeGeometry.AnalyzeGeometry.**AnalyzeGeometry**(*verbose=False*)

Wrapper class for running clashscore

Note: Sequence is required to get the length to calculate % of corrent residues.

---

cleanup()

run(*name*, *verbose=False*)

Parameters

- **name** (*str*) – the path of the file to wrap
- **verbose** (*boolen*) – be verbose

Returns

score; % of Backbone torsion suites (# of them per seq)

Return type

float

Output:

```
----------Backbone torsion suites----------

  Suite ID                suite  suiteness  triaged angle
     A A   3                 !!      0.000     delta
     G A   4                 !!      0.000  epsilon-1
     G A  11                 !!      0.000      None
     C A  20                 !!      0.000     gamma
     U A  25                 !!      0.000     delta
     A A  26                 !!      0.000   delta-1
     A A  29                 !!      0.000      None
     U A  30                 !!      0.000  epsilon-1
     G A  41                 !!      0.000     delta
     U A  42                 !!      0.000   delta-1
     A A  45                 !!      0.000     delta
     U A  46                 !!      0.000  epsilon-1
     U A  47                 !!      0.000   delta-1
  11 suites triaged and 0 incomplete leaving 35 suites
  13/46 suite outliers present
  Average suiteness: 0.490
13 # count lines after 'traged angle' and minus 3 (# of last lines)
test/1xjrA_M1.pdb
34.7826
```

Output for a perfect structure:

```
/Applications/phenix-1.18.2-3874/build/bin/phenix.rna_validate /Users/magnus/
↪work/src/rna-tools/rna_tools/input/mq/5e3hBC.pdb
CGACGCUAGCGUACGCUAGCGUCG
AnalyzeGeomtery:: ----------Backbone bond lenths----------
```

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```
All bonds within 4.0 sigma of ideal values.

                  ----------Backbone bond angles----------

All angles within 4.0 sigma of ideal values.

                      ----------Sugar pucker----------

All puckers have reasonable geometry.

                ----------Backbone torsion suites----------

0 suites triaged and 0 incomplete leaving 24 suites
All RNA torsion suites are reasonable.
Average suiteness: 0.766
```

rna_tools.tools.mq.AnalyzeGeometry.AnalyzeGeometry.**main**()

4.10 RNA 3D structure prediction

4.10.1 ROSETTA

A set of wrappers around Rosetta (https://www.rosettacommons.org/), mostly based on C. Y. Cheng, F. C. Chou, and R. Das, Modeling complex RNA tertiary folds with Rosetta, 1st ed., vol. 553. Elsevier Inc., 2015. http://www.sciencedirect.com/science/article/pii/S0076687914000524

4.10.1.1 Run (modeling)

rna_rosetta_run.py

rna_rosetta_run.py - prepare & run ROSETTA simulations

Based on C. Y. Cheng, F. C. Chou, and R. Das, Modeling complex RNA tertiary folds with Rosetta, 1st ed., vol. 553. Elsevier Inc., 2015. http: // www.sciencedirect.com / science / article / pii / S0076687914000524

The script makes(1) a folder for you job, with seq.fa, ss.fa, input file is copied as input.fa to the folder(2) make helices(3) prepare rosetta input files(4) sends jobs to the cluster.

The header is take from the fast file(`` > /header / ``) not from the filename of your Fasta file.

I discovered this:

```
qstat -xml | tr '\n' ' ' | sed 's#<job_list[^>]*>#\n#g' \
```

> | sed 's#<[^>]*>##g' | grep " " | column -t

(https://stackoverflow.com/questions/26104116/qstat-and-long-job-names) so there is now need to shorted my job ids.

Helix

Run:

```
rna_rosetta_run.py -i -e -r -g -c 200 cp20.fa
```

-i:

```
# prepare a folder for a run
>cp20
AUUAUCAAGAAUCUCAAAGAGAGAUAGCAACCUGCAAUAACGAGCAAGGUGCUAAAAUAGAUAAGCCAAAUUCAAUUGGAAAAAAUGUUAA
.(((((....(((((.....)))))(((..(((((..[[[[..)).))).))).....)))))..((((......))))......
↪]]]].

[peyote2] ~ rna_rosetta_run.py -i cp20.fa
run rosetta for:
cp20
AUUAUCAAGAAUCUCAAAGAGAGAUAGCAACCUGCAAUAACGAGCAAGGUGCUAAAAUAGAUAAGCCAAAUUCAAUUGGAAAAAAUGUUAA
.(((((....(((((.....)))))(((..(((((..[[[[..)).))).))).....)))))..((((......))))......
↪]]]].
/home / magnus // cp20 / created
Seq & ss created
```

Troubleshooting.

If one of the helices is missing you will get:

```
IOError: [Errno 2] No such file or directory: 'helix1.out'
rosetta_submit.py README_FARFAR o 500 100 taf
Could not find:  README_FARFAR
```

and the problem was a1 and g8 pairing:

```
outputting command line to:  helix0.RUN  # previous helix #0
Sequence:  AUGG CCGG
Secstruc:  ((()))
Not complementary at positions a1 and g8!
Sequence:  GUGGG CCCAU
Secstruc:  (((()())))

Writing to fasta file:  helix2.fasta  # next helix #2
```

My case with a modeling of rp12

> Sequence: cc gc Secstruc: (()) Not complementary at positions 1 and 4!

edit the secondary structure, run the program with -i(init, to overwrite seq.fa, ss.fa) and then it works.

Notes:

```
rp17hc 6 characters
```

```
usage: rna_rosetta_run.py [-h] [-i] [-e] [-r] [-g] [-m MOTIF] [-n NSTRUC]
                          [-c CPUS] [--sandbox SANDBOX]
                          file
```

file
: file: > a04 UAUAACAUAUAAUUUUGACAAUAUGGGUCAUAAGUUUCUACCGGAAUACCGUAAAUAU-UCUGACUAUGUAUA ((((.((((…((.((((…….)))).)).……..(.(((((…….))))).)..))))))))

-h, --help
: show this help message and exit

-i, --init
: prepare _folder with seq and ss

-e, --helices
: produce h(E)lices

-r, --rosetta
: prepare rosetta files (still you need *go* to send jobs to a cluster)

-g, --go
: send jobs to a cluster(run qsubMINI)

-m <motif>, **--motif** <motif>
: include a motif file, e.g. -s E-loop_1q9a_mutated_no_flanks_renumber.pdb

-n <nstruc>, **--nstruc** <nstruc>
: # of structures you want to get

-c <cpus>, **--cpus** <cpus>
: # of cpus to be used

--sandbox <sandbox>
: where to run it (default: RNA_ROSETTA_RUN_ROOT_DIR_MODELING

rna_rosetta_run.py - prepare & run ROSETTA simulations

Based on C. Y. Cheng, F. C. Chou, and R. Das, Modeling complex RNA tertiary folds with Rosetta, 1st ed., vol. 553. Elsevier Inc., 2015. http: // www.sciencedirect.com / science / article / pii / S0076687914000524

The script makes(1) a folder for you job, with seq.fa, ss.fa, input file is copied as input.fa to the folder(2) make helices(3) prepare rosetta input files(4) sends jobs to the cluster.

The header is take from the fast file(`` > /header / ``) not from the filename of your Fasta file.

I discovered this:

```
qstat -xml | tr '\n' ' ' | sed 's#<job_list[^>]*>#\n#g' \
```

> | sed 's#<[^>]*>##g' | grep " " | column -t

(https://stackoverflow.com/questions/26104116/qstat-and-long-job-names) so there is now need to shorted my job ids.

Helix

Run:

```
rna_rosetta_run.py -i -e -r -g -c 200 cp20.fa
```

-i:

```
# prepare a folder for a run
>cp20
AUUAUCAAGAAUCUCAAAGAGAGAUAGCAACCUGCAAUAACGAGCAAGGUGCUAAAAUAGAUAAGCCAAAUUCAAUUGGAAAAAAUGUUAA
.(((((....(((((.....)))))(((..(((((..[[[[..)).)))..)))......)))))..((((......))))........
↪]]]].

[peyote2] ~ rna_rosetta_run.py -i cp20.fa
run rosetta for:
cp20
AUUAUCAAGAAUCUCAAAGAGAGAUAGCAACCUGCAAUAACGAGCAAGGUGCUAAAAUAGAUAAGCCAAAUUCAAUUGGAAAAAAUGUUAA
.(((((....(((((.....)))))(((..(((((..[[[[..)).)))..)))......)))))..((((......))))........
↪]]]].
/home / magnus // cp20 / created
Seq & ss created
```

Troubleshooting.

If one of the helices is missing you will get:

```
IOError: [Errno 2] No such file or directory: 'helix1.out'
rosetta_submit.py README_FARFAR o 500 100 taf
Could not find:  README_FARFAR
```

and the problem was a1 and g8 pairing:

```
outputting command line to:  helix0.RUN  # previous helix #0
Sequence:  AUGG CCGG
Secstruc:  ((()))
Not complementary at positions a1 and g8!
Sequence:  GUGGG CCCAU
Secstruc:  (((()))))

Writing to fasta file:  helix2.fasta  # next helix #2
```

My case with a modeling of rp12

> Sequence: cc gc Secstruc: (()) Not complementary at positions 1 and 4!

edit the secondary structure, run the program with -i(init, to overwrite seq.fa, ss.fa) and then it works.

Notes:

```
rp17hc 6 characters
```

class rna_tools.tools.rna_rosetta.rna_rosetta_run.**CustomFormatter**(*prog*, *indent_increment=2*, *max_help_position=24*, *width=None*)

rna_tools.tools.rna_rosetta.rna_rosetta_run.**get_parser**()

rna_tools.tools.rna_rosetta.rna_rosetta_run.**go**()

> send jobs to a cluster(run qsubMINI)

rna_tools.tools.rna_rosetta.rna_rosetta_run.**main**()

> Pipeline for modeling RNA

rna_tools.tools.rna_rosetta.rna_rosetta_run.**prepare_folder**(*args*, *header*, *seq*, *ss*, *path*)

Make folder for you job, with seq.fa, ss.fa, input file is copied as input.fa to the folder.

For ss lowercase is needed when used with motifs, otherwise:

```
[peyote2] aa20$ rna_rosetta_run.py -r -m E-loop_1q9a_mutated_no_flanks_renumber_for_
↪acy20.pdb ~/aa20.fa
2019-05-03 21:31:30,842 rpt_config_local.py::<module>::rpt_config_local loading...
run rosetta for:
aa20
UACGUUCAUCAUCCGUUUGGAUGACGGAAGUAAGCGAAAGCUGAAGGAACGCAUG
..(((((.((((((....)))))).[.....(((....))).....)))))]...
rna_denovo_setup.py -fasta seq.fa -secstruct_file ss.fa -cycles 20000 -no_minimize -
↪nstruct 50  -s E-loop_1q9a_mutated_no_flanks_renumber_for_acy20.pdb  -silent␣
↪helix0.out helix1.out helix2.out -input_silent_res 3-7 47-51 9-14 19-24 33-35 40-
↪42

Sequence:  UACGUUCAUCAUCCGUUUGGAUGACGGAAGUAAGCGAAAGCUGAAGGAACGCAUG
Secstruc:  ..(((((.((((((....)))))).[.....(((....))).....)))))]...
aaguagaag
AAGUAGAAG
Traceback (most recent call last):
  File "/home/magnus/opt/rosetta_src_2016.13.58602_bundle/tools/rna_tools/bin//rna_
↪denovo_setup.py", line 170, in <module>
    raise ValueError('The sequence in %s does not match input sequence!!' % pdb)
ValueError: The sequence in E-loop_1q9a_mutated_no_flanks_renumber_for_acy20.pdb␣
↪does not match input sequence!!
rosetta_submit.py README_FARFAR o 200 100 aa20_
Could not find:  README_FARFAR
```

rna_tools.tools.rna_rosetta.rna_rosetta_run.**prepare_helices**()

Make helices(wrapper around 'helix_preassemble_setup.py')

> **Warning:** I think multiprocessing of helixX.run does not work.

rna_tools.tools.rna_rosetta.rna_rosetta_run.**prepare_rosetta**(*header*, *cpus*, *motif*, *nstruc*)

Prepare ROSETTA using rna_denovo_setup.py

cpus is used to calc nstruc per job to get 10k structures per full run:

```
:param nstruc: how many structures you want to obtain
:type nstruc: int
:param nstruct = int:
:type nstruct = int: math.floor(20000 / cpus)
:param motif: motif file; e.g., -s E-loop_1q9a_mutated_no_flanks_renumber.pdb
:param 50:
:type 50: nstruc) = 10k / 200 (cpus
```

4.10.1.2 Get a number of structures

rna_rosetta_n.py

rna_roseta_n.py - show me # of structure in a silent file

Example:

```
$ rna_rosetta_n.py ade.out
21594

$ rna_rosetta_n.py *out
default.out 100
default1.out 200
default2.out 200
default3.out 100
```

```
usage: rna_rosetta_n.py [-h] [-v] [-0] file [file ...]
```

file

ade.out

-h, --help

show this help message and exit

-v, --verbose

-0, --zero

rna_roseta_n.py - show me # of structure in a silent file

Example:

```
$ rna_rosetta_n.py ade.out
21594

$ rna_rosetta_n.py *out
default.out 100
default1.out 200
default2.out 200
default3.out 100
```

rna_tools.tools.rna_rosetta.rna_rosetta_n.**get_no_structures**(*file*)

rna_tools.tools.rna_rosetta.rna_rosetta_n.**get_parser**()

rna_tools.tools.rna_rosetta.rna_rosetta_n.**run**(*f*)

Pipline for modeling RNA.

4.10.1.3 Get a head of a Rosetta silent file

rna_rosetta_n.py

rna_roseta_head.py - get a head of a Rosetta silent file.

Example:

```
$ rna_rosetta_head.py -n 10000 thf.out
# a new file will be created, thf_10000.out
```

Silent file:

```
[peyote2] thf head -n 100 thf.out
SEQUENCE:␣
↪ggagaguagaugauucgcguuaaguguguguguaaugggaugucgucacacaacgaagcgagagcgcggugaaucauugcauccgcucca
SCORE:     score    rna_data_backbone    rna_vdw    rna_base_backbone    rna_backbone_
↪backbone    rna_repulsive    rna_base_pair    rna_base_axis    rna_base_stagger    rna_
↪base_stack    rna_base_stack_axis    rna_rg    atom_pair_constraint    linear_
↪chainbreak       N_WC      N_NWC       N_BS description
REMARK BINARY SILENTFILE
SCORE:  -601.975               0.000     31.113             -16.960                  -
↪3.888           20.501          -302.742          -38.531           -158.004          ␣
↪-80.764              -110.053     23.750                   0.000               33.601␣
↪         32          6          86    S_000001_000
FOLD_TREE  EDGE 1 4 -1  JEDGE 4 85 1  C4   C2   END  EDGE 4 5 -1  EDGE 85 80 -1  EDGE 85␣
↪89 -1  JEDGE 80 40 5  C4   C2   END  EDGE 80 78 -1  EDGE 40 43 -1  EDGE 40 33 -1 ␣
↪JEDGE 33 45 4  C4   C2   END  EDGE 45 54 -1  EDGE 45 44 -1  EDGE 33 20 -1  JEDGE 20 65␣
↪3  C2   C4   END  EDGE 65 67 -1  EDGE 20 17 -1  EDGE 65 63 -1  JEDGE 17 69 2  C4   C2 ␣
↪ END  JEDGE 63 58 6  C4   C2   END  EDGE 17 6 -1  EDGE 58 59 -1  EDGE 63 60 -1  EDGE␣
↪69 77 -1  EDGE 58 55 -1  EDGE 69 68 -1  S_000001_000
RT -0.987743 0.139354 0.0703103 0.135963 0.989404 -0.0509304 -0.0766626 -0.0407466 -0.
↪996224 6.25631 0.103544 0.0647696   S_000001_000
RT -0.98312 0.1587 -0.091045 0.166923 0.981743 -0.0912024 0.074909 -0.10486 -0.991662 5.
↪89962 -1.95819 -0.1075   S_000001_000
RT -0.987645 0.154078 0.0285994 0.153854 0.988044 -0.00989514 -0.0297821 -0.00537275 -0.
↪999542 6.13138 1.047 0.115722   S_000001_000
RT -0.989884 0.140722 0.0180554 0.140036 0.989532 -0.0348618 -0.0227723 -0.0319807 -0.
↪999229 6.21787 0.201588 -0.0264223   S_000001_000
RT -0.988455 0.134013 0.0706914 0.134924 0.990822 0.00825457 -0.0689364 0.0176973 -0.
↪997464 6.19447 0.189237 0.125791   S_000001_000
RT -0.990412 0.138036 0.00546261 0.137927 0.990299 -0.0168644 -0.00773751 -0.0159492 -0.
↪999843 6.25456 0.0842849 -0.0135807   S_000001_000
ANNOTATED_SEQUENCE: g[RGU:LowerRNA:Virtual_Phosphate]gaga[RAD:rna_cutpoint_
↪lower]g[RGU:rna_cutpoint_upper]uagaugauucgcguuaaguguguguguaaugggauguc[RCY:rna_cutpoint_
↪lower]g[RGU:rna_cutpoint_upper]ucacacaacg[RGU:rna_cutpoint_lower]a[RAD:rna_cutpoint_
↪upper]agcg[RGU:rna_cutpoint_lower]a[RAD:rna_cutpoint_upper]gagcgcg[RGU:rna_cutpoint_
↪lower]g[RGU:rna_cutpoint_upper]ugaaucauu[URA:rna_cutpoint_lower]g[RGU:rna_cutpoint_
↪upper]cauccgcucca[RAD:UpperRNA] S_000001_000
Le3nY9smsa4zEMGdvAA+z+e
```

It seems to work:

```
-rw-rw-r--   1 magnus users 474M 2017-08-06 05:25 thf_10000.out
-rw -rw-r--   1 magnus users 947M 2017-08-06 04:54 thf.out

[peyote2] thf rna_rosetta_n.py thf_10000.out
10000
```

```
usage: rna_rosetta_n.py [-h] [-v] [-n NSTRUC] file
```

file

ade.out

-h, **--help**

show this help message and exit

-v, **--verbose**

-n <nstruc>, **--nstruc** <nstruc>

rna_roseta_head.py - get a head of a Rosetta silent file.

Example:

```
$ rna_rosetta_head.py -n 10000 thf.out
# a new file will be created, thf_10000.out
```

Silent file:

```
[peyote2] thf head -n 100 thf.out
SEQUENCE:␣
↪ggagaguagaugauucgcguuaaguguguguguaaugggaugucgucacacaacgaagcgagagcgcggugaaucauugcauccgcucca
SCORE:     score    rna_data_backbone    rna_vdw    rna_base_backbone    rna_backbone_
↪backbone    rna_repulsive    rna_base_pair    rna_base_axis    rna_base_stagger    rna_
↪base_stack    rna_base_stack_axis     rna_rg    atom_pair_constraint    linear_
↪chainbreak       N_WC      N_NWC       N_BS description
REMARK BINARY SILENTFILE
SCORE:  -601.975               0.000     31.113             -16.960                  -
↪3.888           20.501         -302.742          -38.531           -158.004          ␣
↪-80.764              -110.053     23.750                   0.000               33.601␣
↪        32          6         86    S_000001_000
FOLD_TREE  EDGE 1 4 -1  JEDGE 4 85 1  C4   C2   END  EDGE 4 5 -1  EDGE 85 80 -1  EDGE 85␣
↪89 -1  JEDGE 80 40 5  C4   C2   END  EDGE 80 78 -1  EDGE 40 43 -1  EDGE 40 33 -1 ␣
↪JEDGE 33 45 4  C4   C2   END  EDGE 45 54 -1  EDGE 45 44 -1  EDGE 33 20 -1  JEDGE 20 65␣
↪3  C2   C4   END  EDGE 65 67 -1  EDGE 20 17 -1  EDGE 65 63 -1  JEDGE 17 69 2  C4   C2 ␣
↪ END  JEDGE 63 58 6  C4   C2   END  EDGE 17 6 -1  EDGE 58 59 -1  EDGE 63 60 -1  EDGE␣
↪69 77 -1  EDGE 58 55 -1  EDGE 69 68 -1  S_000001_000
RT -0.987743 0.139354 0.0703103 0.135963 0.989404 -0.0509304 -0.0766626 -0.0407466 -0.
↪996224 6.25631 0.103544 0.0647696   S_000001_000
RT -0.98312 0.1587 -0.091045 0.166923 0.981743 -0.0912024 0.074909 -0.10486 -0.991662 5.
↪89962 -1.95819 -0.1075   S_000001_000
RT -0.987645 0.154078 0.0285994 0.153854 0.988044 -0.00989514 -0.0297821 -0.00537275 -0.
↪999542 6.13138 1.047 0.115722   S_000001_000
RT -0.989884 0.140722 0.0180554 0.140036 0.989532 -0.0348618 -0.0227723 -0.0319807 -0.
↪999229 6.21787 0.201588 -0.0264223   S_000001_000
RT -0.988455 0.134013 0.0706914 0.134924 0.990822 0.00825457 -0.0689364 0.0176973 -0.
```

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```
↪997464 6.19447 0.189237 0.125791   S_000001_000
RT -0.990412 0.138036 0.00546261 0.137927 0.990299 -0.0168644 -0.00773751 -0.0159492 -0.
↪999843 6.25456 0.0842849 -0.0135807   S_000001_000
ANNOTATED_SEQUENCE: g[RGU:LowerRNA:Virtual_Phosphate]gaga[RAD:rna_cutpoint_
↪lower]g[RGU:rna_cutpoint_upper]uagaugauucgcguuaaguguguguguaaugggauguc[RCY:rna_cutpoint_
↪lower]g[RGU:rna_cutpoint_upper]ucacacaacg[RGU:rna_cutpoint_lower]a[RAD:rna_cutpoint_
↪upper]agcg[RGU:rna_cutpoint_lower]a[RAD:rna_cutpoint_upper]gagcgcg[RGU:rna_cutpoint_
↪lower]g[RGU:rna_cutpoint_upper]ugaaucauu[URA:rna_cutpoint_lower]g[RGU:rna_cutpoint_
↪upper]cauccgcucca[RAD:UpperRNA] S_000001_000
Le3nY9smsa4zEMGdvAA+z+e
```

It seems to work:

```
-rw-rw-r--   1 magnus users 474M 2017-08-06 05:25 thf_10000.out
-rw -rw-r--   1 magnus users 947M 2017-08-06 04:54 thf.out

[peyote2] thf rna_rosetta_n.py thf_10000.out
10000
```

rna_tools.tools.rna_rosetta.rna_rosetta_head.**get_parser**()

rna_tools.tools.rna_rosetta.rna_rosetta_head.**run**()

Pipline for modeling RNA.

4.10.1.4 Cluster

rna_rosetta_cluster.py

rna_rosetta_cluster.py - cluster silent Rosetta files

A wrapper to ROSETTA tools for RNA modeling

Based on C. Y. Cheng, F. C. Chou, and R. Das, Modeling complex RNA tertiary folds with Rosetta, 1st ed., vol. 553. Elsevier Inc., 2015. http://www.sciencedirect.com/science/article/pii/S0076687914000524

```
rna_rosetta_cluster.py ade_min.out 20000
```

Take n * 0.005 (.5%) of all frames and put them into *selected.out*. Then the tool clusters this *selected.out*.

```
usage: rna_rosetta_cluster.py [-h] [--no_select]
                              [--radius-inc-step RADIUS_INC_STEP]
                              [--limit-clusters LIMIT_CLUSTERS]
                              file n
```

file

ade.out

n

# of total structures

-h, --help

show this help message and exit

--no_select

Don't run selection once again. Use selected.out in the current folder

--radius-inc-step <radius_inc_step>

radius incremental step, default 0.5

--limit-clusters <limit_clusters>

# of clusters

rna_rosetta_cluster.py - cluster silent Rosetta files

A wrapper to ROSETTA tools for RNA modeling

Based on C. Y. Cheng, F. C. Chou, and R. Das, Modeling complex RNA tertiary folds with Rosetta, 1st ed., vol. 553. Elsevier Inc., 2015. http://www.sciencedirect.com/science/article/pii/S0076687914000524

```
rna_rosetta_cluster.py ade_min.out 20000
```

Take n * 0.005 (.5%) of all frames and put them into *selected.out*. Then the tool clusters this *selected.out*.

rna_tools.tools.rna_rosetta.rna_rosetta_cluster.**cluster**(*radius*, *limit_clusters*)

Internal function of cluster_loop: It removes cluster.out first.

rna_tools.tools.rna_rosetta.rna_rosetta_cluster.**cluster_loop**(*ns*, *radius_inc_step*, *limit_clusters*)

Go from radius 1 to get 1/6 of structures of ns (# of selected structures) in the first cluster, then it stops.

rna_tools.tools.rna_rosetta.rna_rosetta_cluster.**extract**()

rna_tools.tools.rna_rosetta.rna_rosetta_cluster.**get_no_structures**(*file*)

rna_tools.tools.rna_rosetta.rna_rosetta_cluster.**get_no_structures_in_first_cluster**(*fn*)

Get # of structures in a silent file.

Parameters

fn (*string*) – a filename to a silent file

Returns

int: # of structures in a silent file

rna_tools.tools.rna_rosetta.rna_rosetta_cluster.**get_parser**()

rna_tools.tools.rna_rosetta.rna_rosetta_cluster.**get_selected**(*file*, *nc*)

Get selected for clustering

rna_tools.tools.rna_rosetta.rna_rosetta_cluster.**run**()

Pipline for modeling RNA

4.10.1.5 Minimize

rna_rosetta_min.py

rna_rosetta_min.py - a script to do minimization

The script takes the number of structures and the analyzed silence file and does the maths.

Job names will be as your silent file preceding with ~, .e.g ~tha.

http://www.sciencedirect.com/science/article/pii/S0076687914000524

```
ade$ rna_rosetta_cluster.py ade.out
```

The first number states how many processors to use for the run, while the second number is 1/6 the total number of previously generated FARNA models. If you are running on a supercomputer that only allows specific multiples of processors, use an appropriate number for the first input.:

```
rosetta_submit.py min_cmdline min_out 1 24
```

rosetta_submit.py min_cmdline min_out [1] [16] The first number states how many processors to use for each line in min_cmdline. Here, enter 1 for the first input so that the total number of processors used will be equal to the number of processors entered with the "-proc" flag in command line [12], above. The second number states the maximum time each job will be allowed to run (walltime). Start the run with the appropriate command listed by the out- put above (e.g., source qsubMPI for the Stampede cluster).

E.g. for 20k silet file, 1/6 will be minimized = 3.3k:

```
parallel_min_setup.py -silent rp21cr62.out -tag rp21cr62_min  -proc 200 -nstruct 3200 -
↪out_folder mo -out_script MINIMIZE " -ignore_zero_occupancy false "
rosetta_submit.py MINIMIZE mo 1 100 m

[peyote2] rp21 easy_cat.py mo
Catting into:  rp21_min.out ... from 200 primary files. Found 3200  decoys.

# on 200 cpus it took around ~30min
```

```
usage: rna_rosetta_min.py [-h] [-g] [-c CPUS] file
```

file
: ade.out

-h, --help
: show this help message and exit

-g, --go

-c <cpus>**, --cpus** <cpus>
: default: 200

rna_rosetta_min.py - a script to do minimization

The script takes the number of structures and the analyzed silence file and does the maths.

Job names will be as your silent file preceding with ~, .e.g ~tha.

http://www.sciencedirect.com/science/article/pii/S0076687914000524


```
ade$ rna_rosetta_cluster.py ade.out
```

The first number states how many processors to use for the run, while the second number is 1/6 the total number of previously generated FARNA models. If you are running on a supercomputer that only allows specific multiples of processors, use an appropriate number for the first input.:

```
rosetta_submit.py min_cmdline min_out 1 24
```

rosetta_submit.py min_cmdline min_out [1] [16] The first number states how many processors to use for each line in min_cmdline. Here, enter 1 for the first input so that the total number of processors used will be equal to the number of processors entered with the "-proc" flag in command line [12], above. The second number states the maximum time

each job will be allowed to run (walltime). Start the run with the appropriate command listed by the out- put above (e.g., source qsubMPI for the Stampede cluster).

E.g. for 20k silet file, 1/6 will be minimized = 3.3k:

```
parallel_min_setup.py -silent rp21cr62.out -tag rp21cr62_min  -proc 200 -nstruct 3200 -
↪out_folder mo -out_script MINIMIZE " -ignore_zero_occupancy false "
rosetta_submit.py MINIMIZE mo 1 100 m

[peyote2] rp21 easy_cat.py mo
Catting into:  rp21_min.out ... from 200 primary files. Found 3200  decoys.

# on 200 cpus it took around ~30min
```

rna_tools.tools.rna_rosetta.rna_rosetta_min.**get_no_structures**(*file*)

Get a number of structures in a silent file

rna_tools.tools.rna_rosetta.rna_rosetta_min.**get_parser**()

rna_tools.tools.rna_rosetta.rna_rosetta_min.**min**(*silent_file*, *take_n*, *cpus*, *go*)

Run parallel_min_setup (to MINIMIZE file), rosetta_submit.py, and qsubMINI.

Fix on the way, qsub files:

```
-out:file:silent mo/0/mo/123/tha_min.out -> -out:file:silent mo/123/tha_min.out
```

I don't know why mo/0/ is there. I might be because of my changes in rosetta_submit.py (?).

rna_tools.tools.rna_rosetta.rna_rosetta_min.**run**()

4.10.1.6 Extract lowscore decoy

rna_rosetta_extract_lowscore_decoys.py

rna_rosetta_extract_lowscore_decoys.py - a simple wrapper to extract_lowscore_decoys.py

To be used in Jupter notebooks and other scripts.

```
usage: rna_rosetta_extract_lowscore_decoys.py [-h] [-v] nstruc file
```

nstruc

# of low score structures to obtained

file

silent file

-h, --help

show this help message and exit

-v, --verbose

be verbose

rna_rosetta_extract_lowscore_decoys.py - a simple wrapper to extract_lowscore_decoys.py

To be used in Jupter notebooks and other scripts.

rna_tools.tools.rna_rosetta.rna_rosetta_extract_lowscore_decoys.**get_parser**()

rna_tools.tools.rna_rosetta.rna_rosetta_extract_lowscore_decoys.**rosetta_extract_lowscore_decoys**(*file*, *nstruc*, *log=True*

4.10.1.7 Check progress

rna_rosetta_cluster.py

rna_rosetta_check_progress.py - check progress for many simulations of Rosetta

Example:

```
[peyote2] rosetta_jobs rna_rosetta_check_progress.py .
         jobs  #curr  #todo  #decoys done
0  ./rp17s223    200      0      407  [ ]
1   ./rp17hcf      0      0        0  [ ]
# curr  232 #todo  0
```

```
usage: rna_rosetta_cluster.py [-h] [-v] [-m] [-s SELECT] [-k] dir
```

dir

directory with rosetta runs, define by RNA_ROSETTA_RUN_ROOT_DIR_MODELING right now:

-h, --help

show this help message and exit

-v, --verbose

be verbose

-m, --min-only

check only for mo folder

-s <select>, **--select** <select>

select for analysis only jobs with this phrase, .e.g., **evoseq_**

-k, --kill

kill (qdel) jobs if your reach limit (nstruc) of structure that you want, right now is 10000 structures

rna_rosetta_check_progress.py - check progress for many simulations of Rosetta

Example:

```
[peyote2] rosetta_jobs rna_rosetta_check_progress.py .
         jobs  #curr  #todo  #decoys done
0  ./rp17s223    200      0      407  [ ]
1   ./rp17hcf      0      0        0  [ ]
# curr  232 #todo  0
```

rna_tools.tools.rna_rosetta.rna_rosetta_check_progress.**get_parser**()

rna_tools.tools.rna_rosetta.rna_rosetta_check_progress.**run_cmd**(*cmd*)

4.10.2 SimRNA

4.10.2.1 Select low energy frames

rna_simrna_lowest.py

rna_simrna_lowest.py - get lowest energy frames out of a SimRNA trajectory file

This code uses heavily the SimRNATrajectory class. Be default 100 lowest energy frames is exported.

```
usage: rna_simrna_lowest.py [-h] [-n NSTRUC] trafl
```

trafl
SimRNA trafl file

-h, --help
show this help message and exit

-n <nstruc>, **--nstruc** <nstruc>
SimRNA trafl file

4.10.2.2 Extract

rna_simrna_extract.py

rna_simrna_extra.py - extract full atom structures from a SimRNA trajectory file

Options:

SIMRNA_DATA_PATH has to be properly defined in `rpt_config_local`.

```
usage: rna_simrna_extract.py [-h] -t TEMPLATE -f TRAFL [-c]
                             [-n NUMBER_OF_STRUCTURES]
```

-h, --help
show this help message and exit

-t <template>, **--template** <template>
template PDB file used for reconstruction to full atom models

-f <trafl>, **--trafl** <trafl>
SimRNA trafl file

-c, --cleanup
Keep only *_AA.pdb files, move *.ss_detected and *.pdbto _<traj name folder>

-n <number_of_structures>, **--number_of_structures** <number_of_structures>

4.10.3 SimRNAweb

4.10.3.1 Download files of a SimRNAweb run

rna_simrnaweb_download_job.py

rna_simrnaweb_download_job.py - download model files, trajectory for a given SimRNAweb job.

Usage:

```
rp17pk$ rna_pdb_download_simrna_job.py 27b5093d -m -t -x
# download more clusters, trajectory, extract100

cp771_pk$ rna_pdb_download_simrna_job.py -t -x -m cf8f8bb2 -p cp771_pk
# download with a trajectory, and cluster #4 and #5, add to all pdb files
# prefix: cp771_pk

$ rna_simrnaweb_download_job.py --web-models rp17_well_d10_e1-a43d3ab5 --prefix tar
# prefix added will be tar_XXXX
```

Example:

```
rna_pdb_download_simrna_job.py -t -x -m 20569fa1 -p zmp_pk

[mm] zmp_pk ls
20569fa1_ALL_100low.trafl
_20569fa1-thrs7.10A_clust04
_20569fa1-thrs7.10A_clust05
_20569fa1_ALL_100low
data
rna_simrna_extract.log
subset.png
zmp_pk_20569fa1-thrs7.10A_clust01X.pdb
zmp_pk_20569fa1-thrs7.10A_clust02X.pdb
zmp_pk_20569fa1-thrs7.10A_clust03X.pdb
zmp_pk_20569fa1-thrs7.10A_clust04X.pdb
zmp_pk_20569fa1-thrs7.10A_clust05X.pdb
```

```
usage: rna_simrnaweb_download_job.py [-h] [-p PREFIX] [-n NSTRUC] [-e] [-m]
                                     [-r] [-c] [-d] [--top100] [--top200]
                                     [--web-models]
                                     job_id
```

job_id

job_id

-h, --help

show this help message and exit

-p <prefix>, **--prefix** <prefix>

prefix to the name, withouth _, be careful with this.If you have already some files with the given folder, their names mightbe changed.

-n <nstruc>, **--nstruc** <nstruc>

extract nstruc the lowest energy, this option must go with –web

-e, --extract
extract nstruc the lowest energy, this option must go with –web

-m, --more_clusters
download also cluster 4 and 5

-r, --remove-trajectory
remove trajectory after analysis

-c, --cluster
get trajectory from cluster OR local on your computer (mdfind for macOS)

-d, --download-trajectory
web

--top100
download top100 trajectory

--top200
download top200 trajectory

--web-models
web models download

4.10.4 SimRNATrajectory

SimRNATrajectory module.

SimRNATrajectory / Frame / Residue / Atom

class rna_tools.tools.simrna_trajectory.simrna_trajectory.**Atom**(*name*, *x*, *y*, *z*)
x y z coord

get_coord()
Return coords (np.array).

class rna_tools.tools.simrna_trajectory.simrna_trajectory.**Frame**(*id*, *header*, *coords*, *top_level=False*)

Syntax of header:

- write_number
- replica_id
- total_energy
- energy_without_restraints
- temperature

> **Warning:** If there is an invalid frame, please use *repair_traﬂ.py* to fix the trajectory first.

rmsd_to(*frame*, *verbose=False*)

class rna_tools.tools.simrna_trajectory.simrna_trajectory.**Residue**(*id*, *p*, *c4p*, *n1n9*, *b1*, *b2*)

Create Residue object.

Each residue in SimRNA coarse-grained represantation consists only 5 coarse-grained atoms:

- backbone: p = phospate group, c4p = sugar moiety
- nucleotide: n1n9 = N1 for pyrimidines, N9 for purines, b1 = C2 for purines and pyrimidines, b2 = C4 for pyrimidines, C6 for purines

get_atoms()

Return all atoms

get_center()

Return MB for residue `((self.n1n9 + self.b2) / 2)`

class rna_tools.tools.simrna_trajectory.simrna_trajectory.**SimRNATrajectory**

load_from_file(*fn*, *debug_break=False*, *top_level=False*, *only_first_frame=False*)

Create a trajectory based on give filename.

Parameters

top_level – top_level = True, don't make a huge tree of objects (Residues/Atoms) == amazing speed up! Useful if you need only frames, energies and coords as text. You only get the info that is in header of each frame.

top_level = False, makes huge tree of objects (Residues/Atoms) == very slow for a huge trajectories

Warning: Loads up whole trafl file into memory, and get stuck. Use this if you want to compute e.g. distances between atoms, get the positions of specified atoms etc. If you can not process your trajectory

use top_level=True or look at load_from_string() to load a frame by frame from a file.

h(eader), l(line), f(ile)

load_from_list(*frames*)

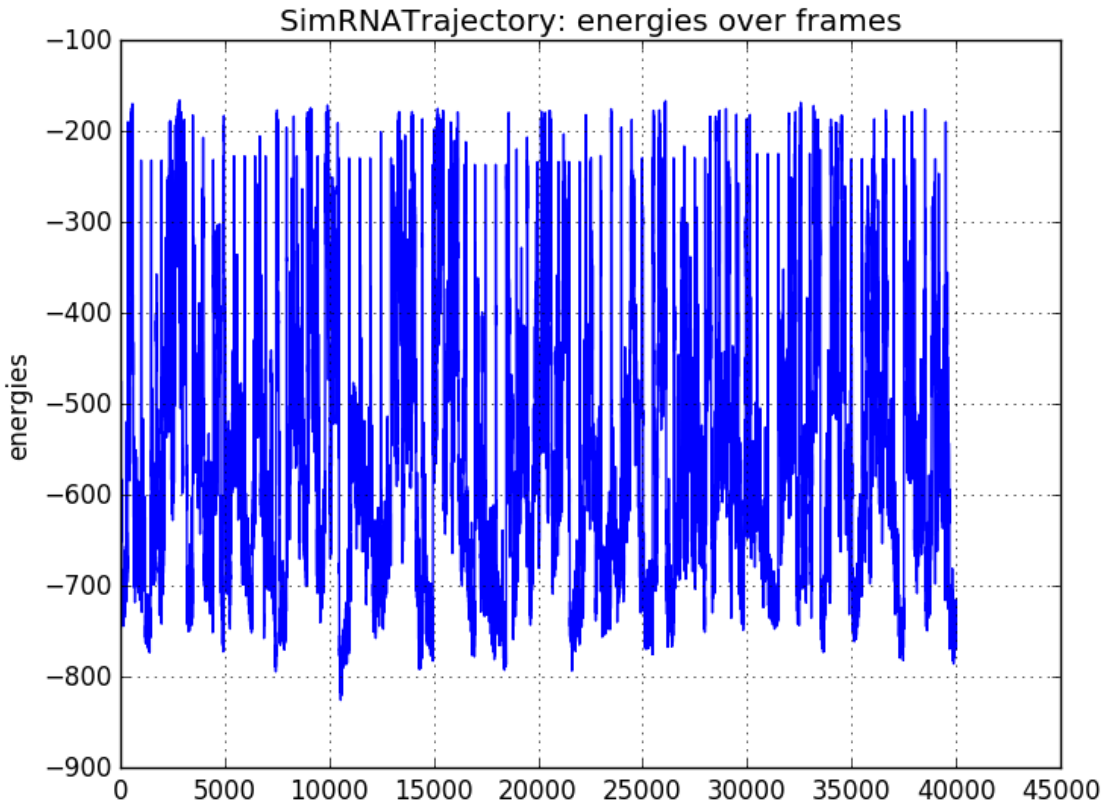
load_from_string(*c*, *txt*)

Create a trajectory based on given string (txt) with id given by c.

Faster method, loads only one frame at a time to memory, and after computations loads the next frame (memory efficient).

plot_energy(*plotfn='plot.png'*)

Plots the SimRNA energy of the trajectory.



save(*fn*, *verbose=True*)

Save the trajectory to file.

sort(*inplace=True*)

Sort frames within the trajectory according to energy.

4.11 RNA Refinement (QRNAS)

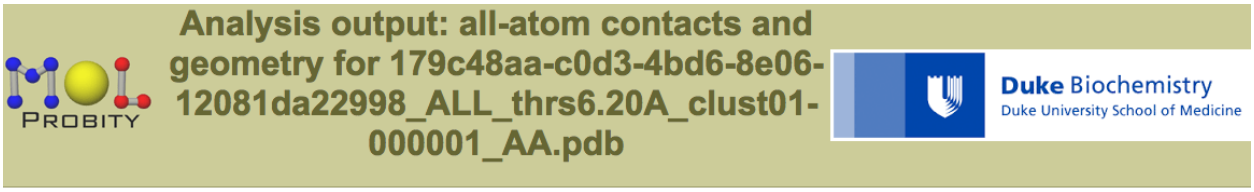
4.11.1 rna_refinement.py

rna_refinement - RNA refinement with QRNAS.

Models of RNA 3D structures obtained by modeling methods often suffer from local inaccuracies such as clashes or physically improbable bond lengths, backbone conformations, or sugar puckers. To ensure high quality of models, a procedure of re nement should be applied as a nal step in the modeling pipeline. The software tool QRNAS was developed in our laboratory to perform local re nement of nucleic acid structures based on an extended version of the AMBER force field. The extensions consist of energy terms associated with introduction of explicit hydrogen bonds, idealization of base pair planarity and regularization of backbone conformation.

Read more: Piatkowski, P., Kasprzak, J. M., Kumar, D., Magnus, M., Chojnowski, G., & Bujnicki, J. M. (2016). RNA 3D Structure Modeling by Combination of Template-Based Method ModeRNA, Template-Free Folding with SimRNA, and Refinement with QRNAS. Methods in Molecular Biology (Clifton, N.J.), 1490(Suppl), 217-235. http://doi.org/10.1007/978-1-4939-6433-8_14

Right now, there is 20k steps of refinement.

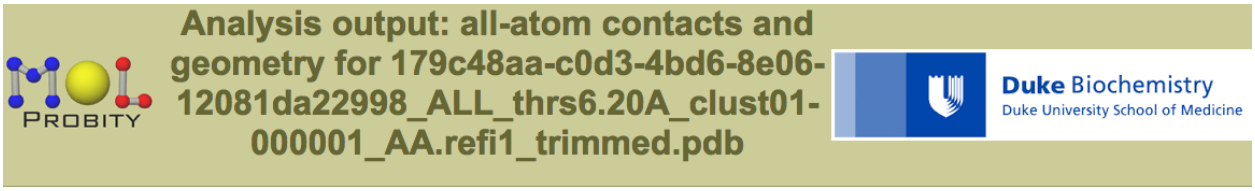


Summary statistics

All-Atom Contacts	Clashscore, all atoms:	176.47		0th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Nucleic Acid Geometry	Probably wrong sugar puckers:	4	6.45%	Goal: 0
	Bad backbone conformations#:	21	33.87%	Goal: <= 5%
	Bad bonds:	60 / 1481	4.05%	Goal: 0%
	Bad angles:	161 / 2306	6.98%	Goal: <0.1%

In the two column results, the left column gives the raw count, right column gives the percentage.
* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.
# RNA backbone was recently shown to be rotameric. Outliers are RNA suites that don't fall into recognized rotamers.

The initial structure, `179c48aa-c0d3-4bd6-8e06-12081da22998_ALL_thrs6.20A_clust01-000001_AA.pdb`.

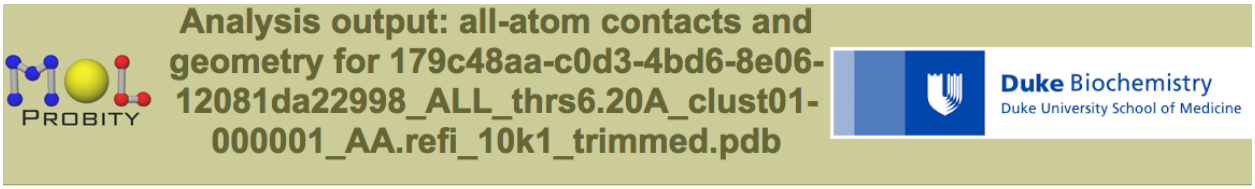


Summary statistics

All-Atom Contacts	Clashscore, all atoms:	66.7		1st percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Nucleic Acid Geometry	Probably wrong sugar puckers:	7	11.29%	Goal: 0
	Bad backbone conformations#:	20	32.79%	Goal: <= 5%
	Bad bonds:	24 / 1458	1.65%	Goal: 0%
	Bad angles:	235 / 2270	10.35%	Goal: <0.1%

In the two column results, the left column gives the raw count, right column gives the percentage.
* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.
# RNA backbone was recently shown to be rotameric. Outliers are RNA suites that don't fall into recognized rotamers.

after 3k, ~10min

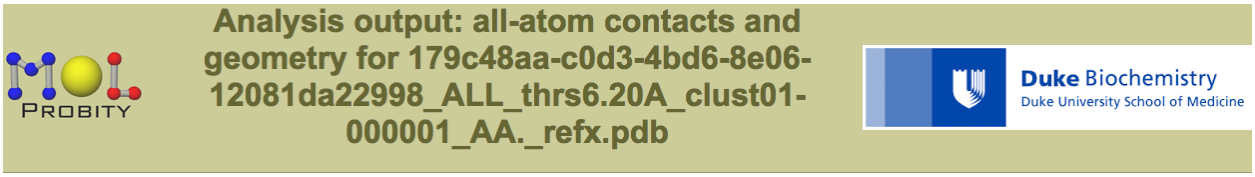


Summary statistics

All-Atom Contacts	Clashscore, all atoms:	2.02		99th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Nucleic Acid Geometry	Probably wrong sugar puckers:	7	11.29%	Goal: 0
	Bad backbone conformations#:	15	24.59%	Goal: <= 5%
	Bad bonds:	2 / 1458	0.14%	Goal: 0%
	Bad angles:	35 / 2270	1.54%	Goal: <0.1%

In the two column results, the left column gives the raw count, right column gives the percentage.
* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.
# RNA backbone was recently shown to be rotameric. Outliers are RNA suites that don't fall into recognized rotamers.

after 10k steps, around 30min



Summary statistics

All-Atom Contacts	Clashscore, all atoms:	4.02		96th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Nucleic Acid Geometry	Probably wrong sugar puckers:	6	9.68%	Goal: 0
	Bad backbone conformations#:	12	19.67%	Goal: <= 5%
	Bad bonds:	1 / 1458	0.07%	Goal: 0%
	Bad angles:	17 / 2270	0.75%	Goal: <0.1%

In the two column results, the left column gives the raw count, right column gives the percentage.
* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.
# RNA backbone was recently shown to be rotameric. Outliers are RNA suites that don't fall into recognized rotamers.

after 20k steps, around 1h.

Installation of QRNAS

Download the QRNAS package from http://genesilico.pl/qrnas/, unzip the archive, and compile it with the following command:

```
./qrnamake sequential
```

This should create an executable version of QRNAS.

> **Warning:** Please, change the name of the binary file from QRNA to QRNAS!

Be default the script searches QRNAS in <rna-tools>/opt/qrnas/ .

Usage of QRNA:

```
QRNA - Quick Refinement of Nucleic Acids (0.2 alpha)
     by Juliusz Stasiewicz (jstasiewicz@genesilico.pl)

To use type:
  QRNA -i <input PDBfile> [-o <output PDBfile>] [-c <configfile>] [-p] [-m
↪<restraintsfile>]
OR specify <input PDBfile>, <output PDBfile> and <restraintsfile> in <configfile> and␣
↪type just:
  QRNA -c <configfile>
```

Installation of this util

Set up in your bashrc:

```
export QRNAS_PATH=<your path to qrnas> # e.g. /home/magnus/src/rna-tools/opt/qrnas
```

but default rna-tools searches for qrnas in <rna-tools>/opt/qrnas.

QRNAS at Peyote2

There is no problem to run QRNAS at our Genesilico cluster, *peyote2*. Tested by mmagnus –170822. Copy files of QRNAS to peyote and run `./qrnamake sequential`.

To run it at a cluster with the Sun Grid Engine queuing system (this one with qusb ;-)):

```
for p in *.pdb; do echo "rna_refinement.py $p >& ${p}.log" | qsub -cwd -V -pe mpi 1 -N
↪"r_$p" ; done
```

DONE:

- [x] clean up the output structure
- [x] configuration should not be hardcoded

```
usage: rna_refinement.py [-h] [-s STEPS] [-o OUTPUT_FILE] [-i] [-v] fn
```

fn
: input pdb file

-h, --help
: show this help message and exit

-s <steps>, **--steps** <steps>
: # of steps, default: 20k

-o <output_file>, **--output_file** <output_file>
: output pdb file

-i, --interactive

-v, --verbose

4.12 RNA Molecular Dynammics (MD)

4.13 diffpdb

diffpdb - a simple tool to compare text-content of PDB files

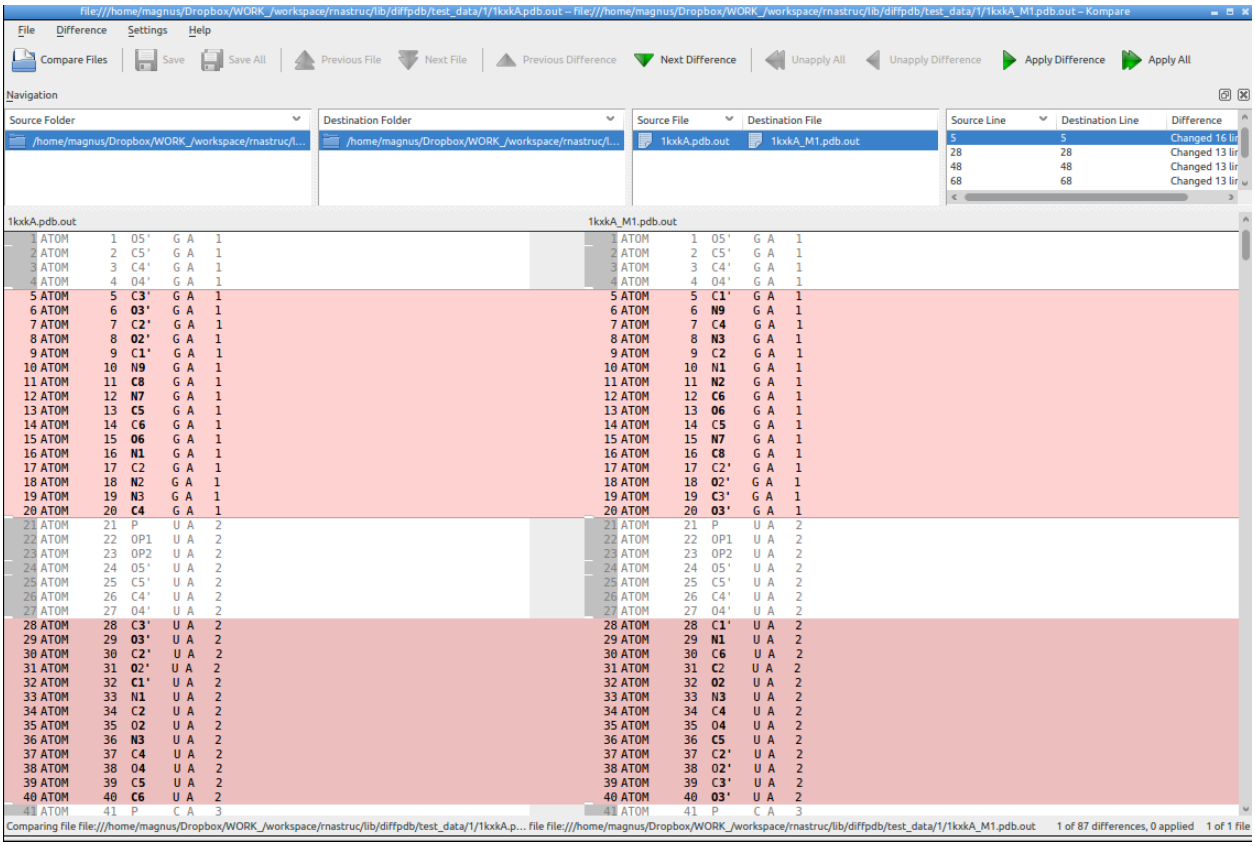
The method is quick-and-dirty, but works!

The script takes first 31 characters of lines (or only atom names and residue names) starting with `HETATM` or `ATOM` and save these lines to a <filename>.out file.

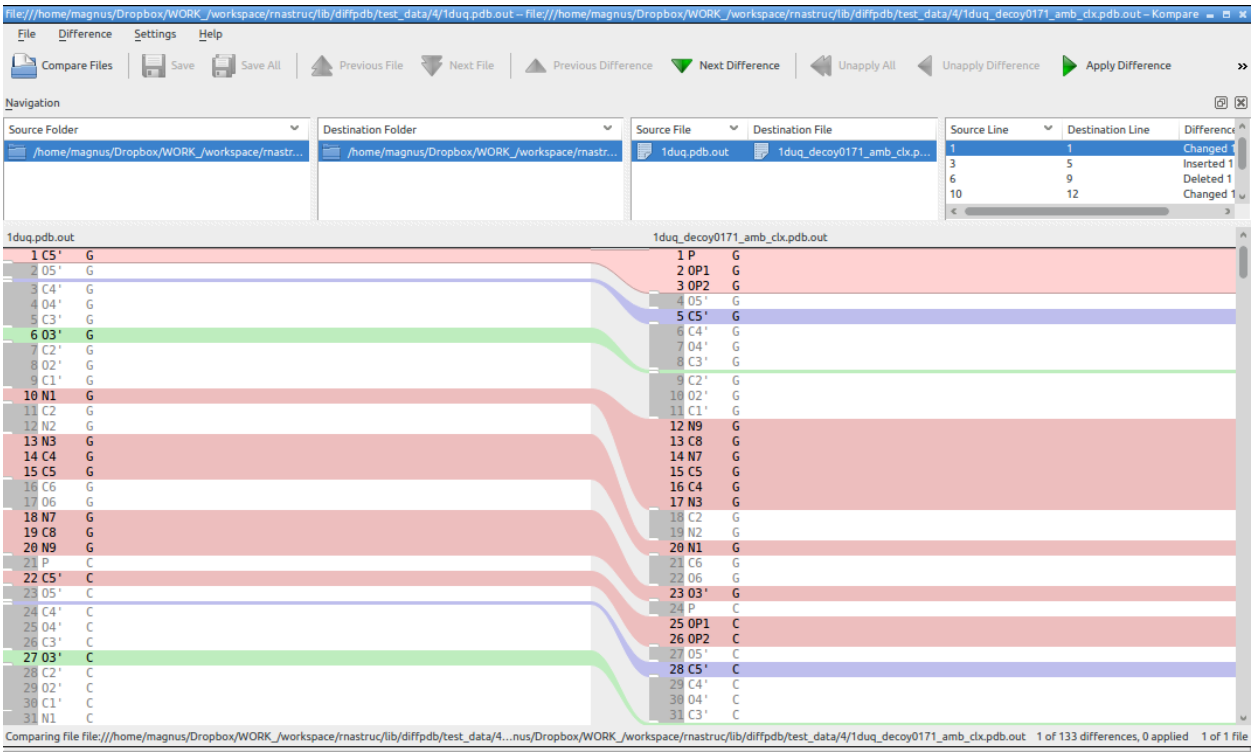
One file is created per pdb. In the final step DIFF_TOOL is executed on these two output files. You get a diff output. That's it! Enjoy!

Configuration:

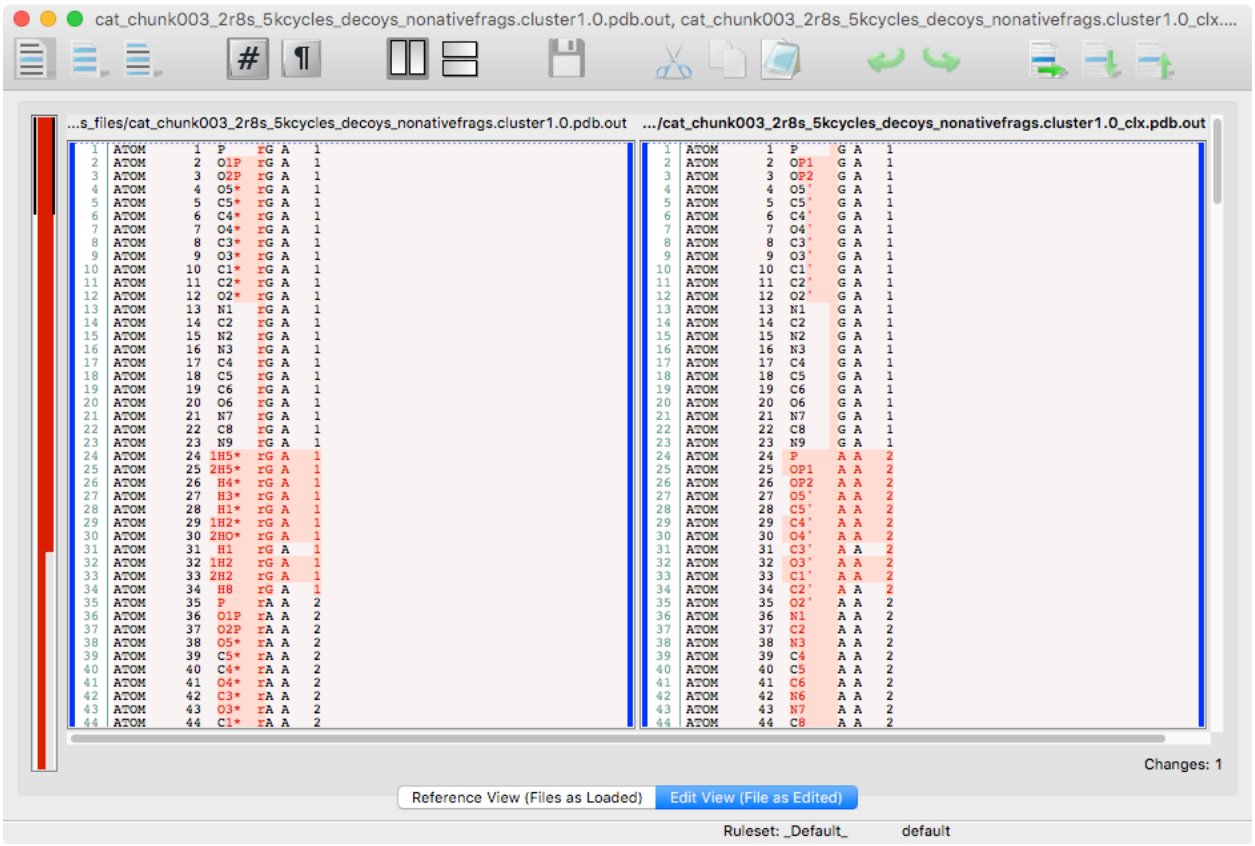
- `DIFF_TOOL="open -a diffmerge"` or `DIFF_TOOL="kompare"` to set up what tool would you like to use to diff files in the file `rna-pdb-tools/tools/diffpdb/diffpdb_conf.py` (create it if needed)



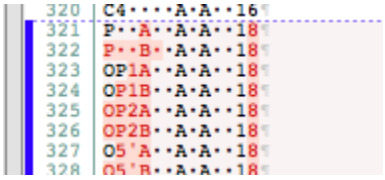

```
./diffpdb.py --names test_data/4/1duq.pdb test_data/4/1duq_decoy0171_amb_clx.pdb
```



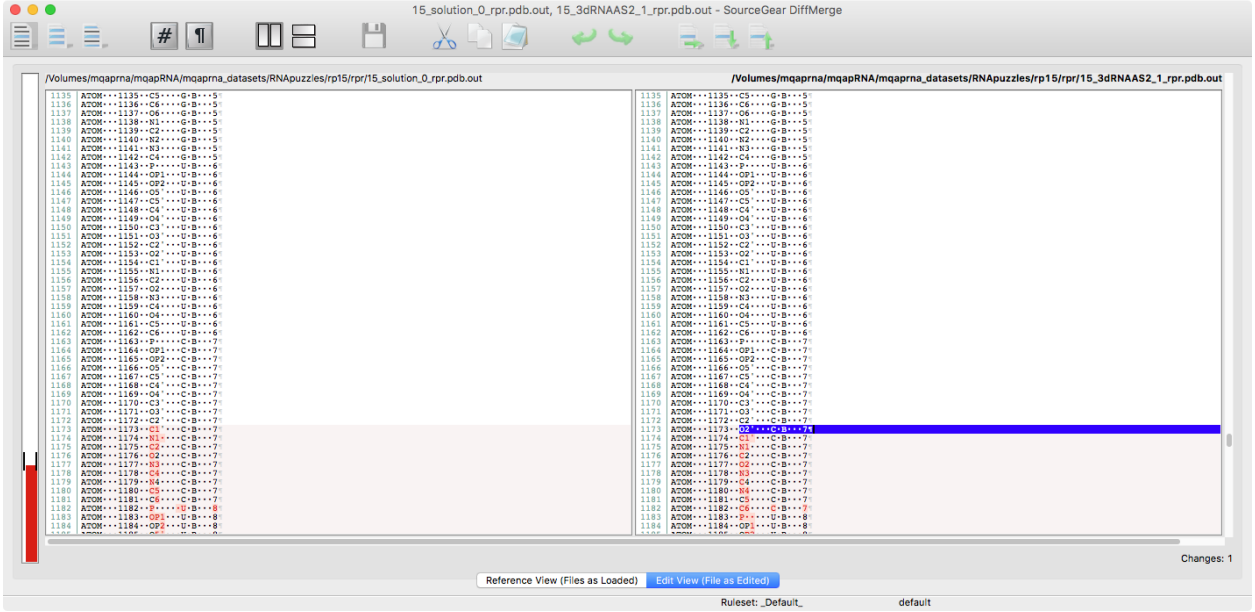
and on the Mac (using `diffmerge`):



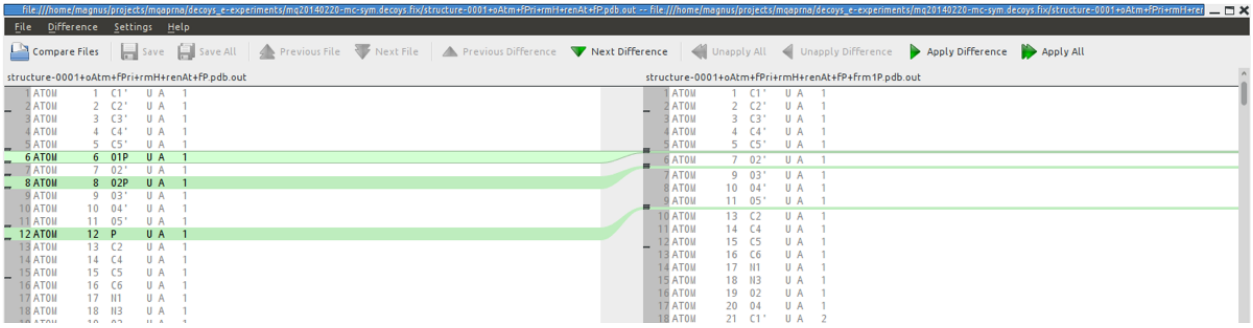
One of the difference that can be detected with the script is variants of atoms.



or a detection of missing atom.



or a detection of missing OP3 at the beginning.



4.14 RNA clustering with CLANS (clanstix)

rna_clanstix - a tool for visualizing RNA 3D structures based on pairwise structural similarity with Clans.

We hacked Clans thus instead of BLAST-based distances between sequences, you can analyze distances between structures described as p-values of rmsd (based on the method from the Dokholyan lab.)

Quickref:

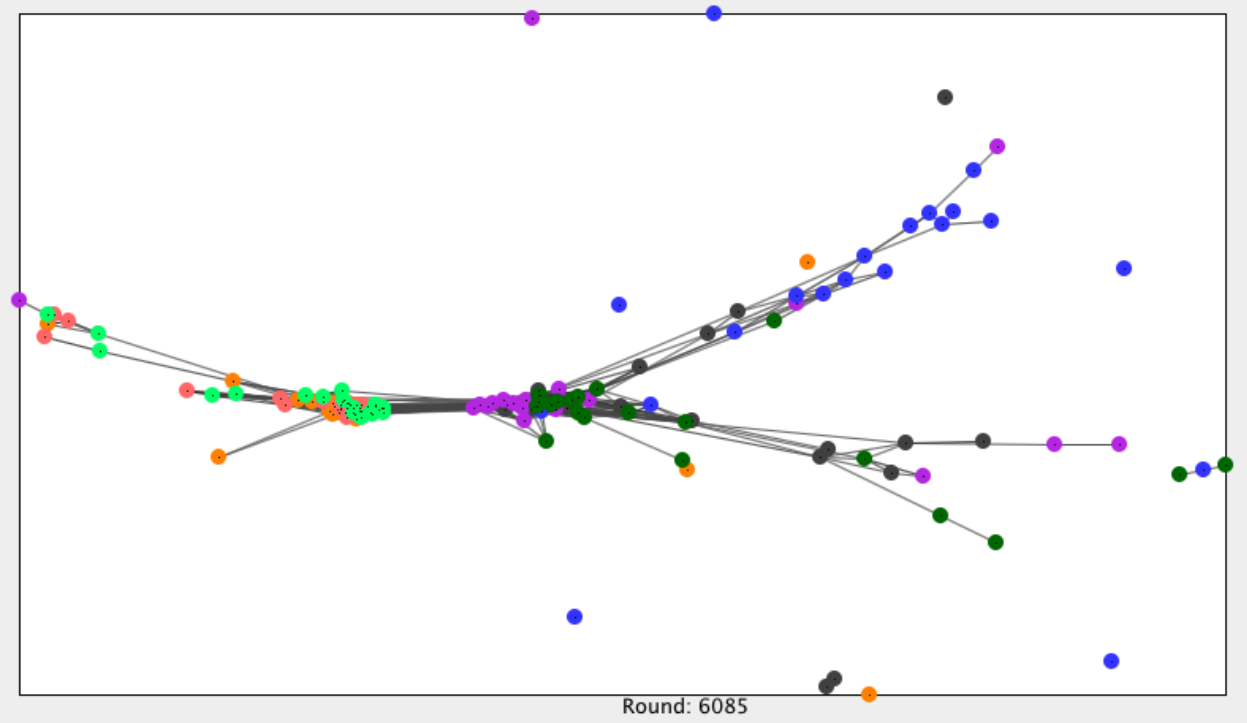
```
rna_clanstix.py --groups-auto 10 --color-by-homolog --shape-by-source  thf_ref_mapping_
↪pk_refX.txt input2.clans
```

Running Clans: To run CLANS you need to have Java 1.4 or better installed (java can be downloaded HERE). For full functionality you will also need the NCBI BLAST,PSI-BLAST and formatdb executables (NCBI). For command line parameters and basic help please refer to the README file. (source: http://www.eb.tuebingen.mpg.de/research/departments/protein-evolution/software/clans.html)

The RMSDs between structures are converted into p-values based on the method from the Dokholyan lab or some hacky way developed by mmagnus .

4.14.1 Color groups

You can color your groups:



To get colors, run a cmd like this:

```
rna_clastix.py rnapz17_matrix_farfar_HelSeedCst.txt --groups␣
↪20:seq1+20+20+20+20+20+20:seq10
```

where with the + sign you separate groups. Each group has to have a number of structures. Optionally it can have a name, e.g., `20:seq1`, use `:` as a separator. If a provided name is `native` then this group will be shown as starts.

Get inspiration for more colors (http://www.rapidtables.com/web/color/RGB_Color.htm)

4.14.2 How to use ClanstixRNA?

1. Get a matrix of distances, save it as e.g. matrix.txt (see Comment below)
2. run ClanstixRNA on this matrix to get an input file to Clans (e.g. clans_rna.txt):

   ```
   rna_clanstix.py test_data/matrix.txt # clans.input will be created by default
   ```

3. open CLANS and click File -> Load run and load clans_run.txt
4. You're done! :-)

Comment: To get this matrix you can use for example another tool from the rna-pdb-tools packages:

```
rna_calc_rmsd_all_vs_all.py -i rp18 -o rp18_rmsd.csv
rna_clastix.py --groups 1:native+5:3dRNA+
      5:Chen+3:Dokh+5:Feng+5:LeeASModel+
      5:Lee+5:RNAComposer+10:RW3D+5:Rhiju+
```

(continues on next page)

(continued from previous page)

```
      1:YagoubAli+3:SimRNA  rp18_rmsd.csv clans.in

rna_clastix.py --groups 100+100+100+100+100+100+100+100+100+100+1:native  rp18_rmsd.csv
```

where `rp18` is a folder with structure and `rp18_rmsd.csv` is a matrix of all-vs-all rmsds.

Hajdin, C. E., Ding, F., Dokholyan, N. V, & Weeks, K. M. (2010). On the significance of an RNA tertiary structure prediction. RNA (New York, N.Y.), 16(7), 1340–9. doi:10.1261/rna.1837410

An output of this tool can be viewed using CLANS.

Frickey, T., & Lupas, A. (2004). CLANS: a Java application for visualizing protein families based on pairwise similarity. Bioinformatics (Oxford, England), 20(18), 3702–4. doi:10.1093/bioinformatics/bth444

class rna_tools.tools.clanstix.rna_clanstix.**RNAStructClans**(*n=10*, *dotsize=10*)

Clans run.

Usage:

```
>>> f = open('matrix.txt')
>>> ids = f.readline().replace('#','').split()
>>> c = RNAStructClans(n=len(ids)) # 200?
>>> c.add_ids(ids)
>>> c.dist_from_matrix(f)
>>> print(c.txt)
```

add_ids(*ids*)

dist_from_matrix(*rmsds*, *matrix=0*, *use_pv=False*, *use_input_values=False*, *dont_calc=False*, *debug=False*)

dist_from_matrix_mp(*output_pmatrix_fn*, *max*, *min*, *lines*, *pmat=False*, *use_pv=False*, *use_input_values=False*, *debug=False*)

rna_tools.tools.clanstix.rna_clanstix.**check_symmetric**(*a*, *rtol=1e-05*, *atol=1e-08*)

https://stackoverflow.com/questions/42908334/checking-if-a-matrix-is-symmetric-in-numpy

rna_tools.tools.clanstix.rna_clanstix.**get_parser**()

4.15 Misc

4.15.1 Plotting

4.15.1.1 rna_plot_hist.py

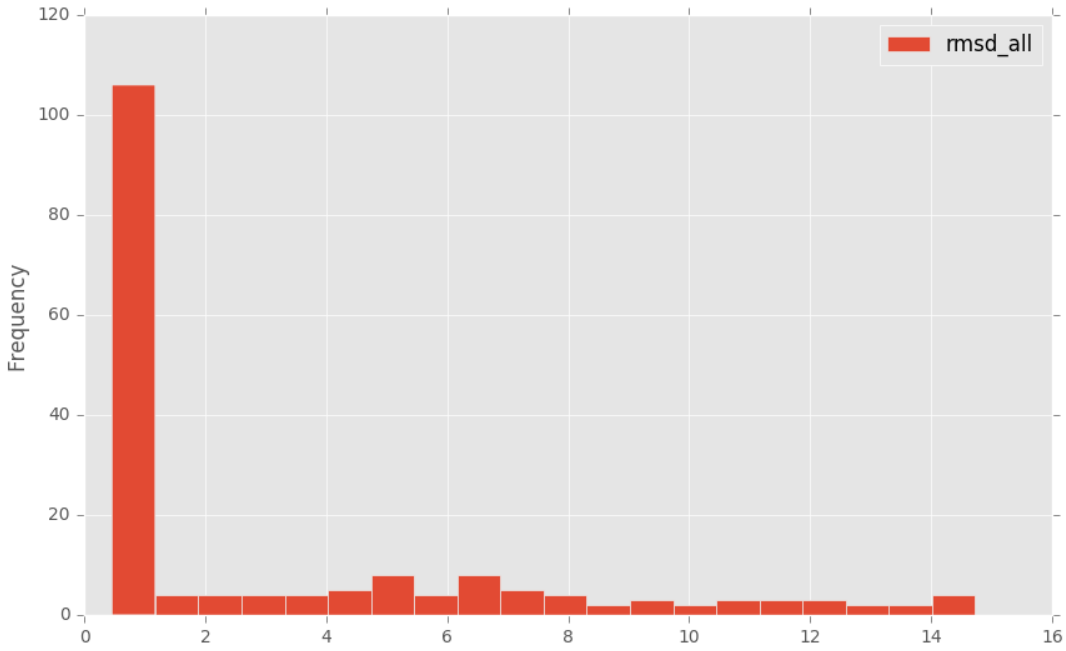
rna_plot_hist.py - generate a histogram

Don't open Excel, Jupyter. Simple plot a histogram of one column and save it to a file.

Example:

```
# file
                                                fn  rmsd_all
0  19_Bujnicki_Human_4_rpr_n0-000001.pdb-000001_A...     14.73
1  19_Bujnicki_Human_4_rpr_n0-000001.pdb.trafl_19...      0.46
2  19_Bujnicki_Human_4_rpr_n0-000001.pdb.trafl_19...     14.73
3  19_Bujnicki_Human_4_rpr_n0-000001.pdb_thrs0.50...      0.73
4  19_Bujnicki_Human_4_rpr_n0-000001.pdb_thrs0.50...      0.83

$ rna_plot_hist.py rmsds.csv --column rmsd_all
```



```
usage: rna_plot_hist.py [-h] [--column COLUMN] [--sep SEP] [-o OUTPUT]
                        [--bins BINS]
                        file
```

file

rmsd.txt

-h, --help

show this help message and exit

--column <column>

column of file to plot

--sep <sep>

separator, be default

-o <output>, **--output** <output>

--bins <bins>

4.15.1.2 rna_plot_density.py

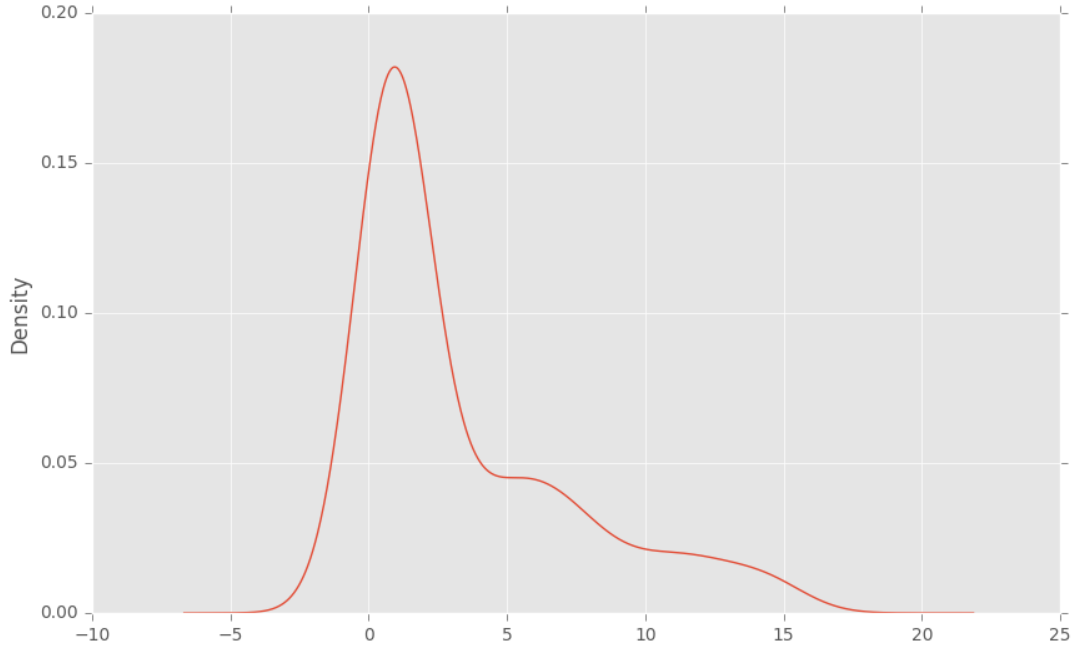
rna_plot_density.py - generate a density plot

Don't open Excel, Jupyter. Simple plot a density of one column and save it to a file.

Example:

```
# file
                                                fn  rmsd_all
0  19_Bujnicki_Human_4_rpr_n0-000001.pdb-000001_A...     14.73
1  19_Bujnicki_Human_4_rpr_n0-000001.pdb.trafl_19...      0.46
2  19_Bujnicki_Human_4_rpr_n0-000001.pdb.trafl_19...     14.73
3  19_Bujnicki_Human_4_rpr_n0-000001.pdb_thrs0.50...      0.73
4  19_Bujnicki_Human_4_rpr_n0-000001.pdb_thrs0.50...      0.83

$ rna_plot_hist.py rmsds.csv --column rmsd_all
```




```
usage: rna_plot_density.py [-h] [--column COLUMN] [--sep SEP] [-o OUTPUT] file
```

file
rmsd.txt

-h, --help
show this help message and exit

--column <column>
column of file to plot

--sep <sep>
separator, be default

-o <output>, **--output** <output>

4.15.2 rna_sali2dotbracket

4.15.2.1 rna_sali2dotbracket

```
usage: rna_sali2dotbracket [-h] filename
```

filename
file in the Sali format

-h, --help
show this help message and exit

This beauty here will go to sali notation and convert it to dotbracket notation. The file name should be xxxx.sali

Author: Catarina Almeida

rna_tools.tools.rna_sali2dotbracket.rna_sali2dotbracket.**convert_sali2dotbracket**(*fn*)

The function needs a filename in the Sali format. This function will get the secondary structure of the sequence, then get its identifier and then the sequence itself.

To get the ss

The line with the secondary structure is a list and will look like this:

```
['', '', '', '', '', '', '', '', '', '', '--...<<<[[...]]..>>>>', '', '', '\n']
```

In this case, the ss is in the 11th position. But in some files it may be in the 12th, 13th, 10th, etc..

If the longest element from the list is extracted, then this problem is overcomed.

The ss will some times have patterns of repeated gaps, which will come in the form of:

a. x

b. xnt

c. (x)

With x being any number, from 1 to 1000. These must be converted to the correspondent number of gaps (-) in the converted ss. This conversion is done by:

1 - Identifying the pattern with regex

2 - Replacing it with repl function.

As such, the following expressions will replace the previously mentioned patterns:

a. `re.sub(r'\d*\d', repl, temp)`

b. `re.sub(r'\d*\dnt', repl, temp)`

c. `re.sub(r'(?P<smthBeautiful>\(\d+\))', repl, temp)`

To get the sequence

The sequence, much like the ss, can sometimes be in a different position in the list. Like in the ss, the longest element will be selected. Also, like in the ss, patterns for repeated gaps appear. So these must also be removed.

rna_tools.tools.rna_sali2dotbracket.rna_sali2dotbracket.**get_parser**()

rna_tools.tools.rna_sali2dotbracket.rna_sali2dotbracket.**repl**(*m*)

This function will replace the length of a given string by the correspondent number of dashes. The expression `qwerty` will be replaced by `-----`.

4.15.3 Cluster load

A very simple tool to see your cluster load per user:

```
MAX_JOBS: 1000
#jobs cluster 917 load:  0.917  to use: 83
#jobs you     749 load:  0.749  to use: 251
{'deepak': 160, 'azyla': 8, 'magnus': 749}
1 azyla        r 8
20 magnus       r 10
16 deepak       r 10
```

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```
329 magnus       r 1
22 magnus       qw 10
```

A super simple script to get some statistics of who is running at a cluster

Set MAX_JOBS to calc % of usage, it's an approximation of max number of jobs, e.g. peyote ~1k (rather 700, e.g. FARNA runs.).

rna_tools.tools.cluster_load.cluster_load.**get_parser**()

rna_tools.tools.cluster_load.cluster_load.**per_user**()

get stats (#cpus) per user

rna_tools.tools.cluster_load.cluster_load.**stats_for_cluster**()

get stats (#jobs) per cluster

rna_tools.tools.cluster_load.cluster_load.**stats_for_user**()

get stats (#jobs) per user

4.15.4 RNAkb

CHAPTER

FIVE

RNA-TOOLS & PYMOL [PYMOL4RNA]

See also https://github.com/mmagnus/rna-tools/tree/master/rna_tools/tools/PyMOL4RNA

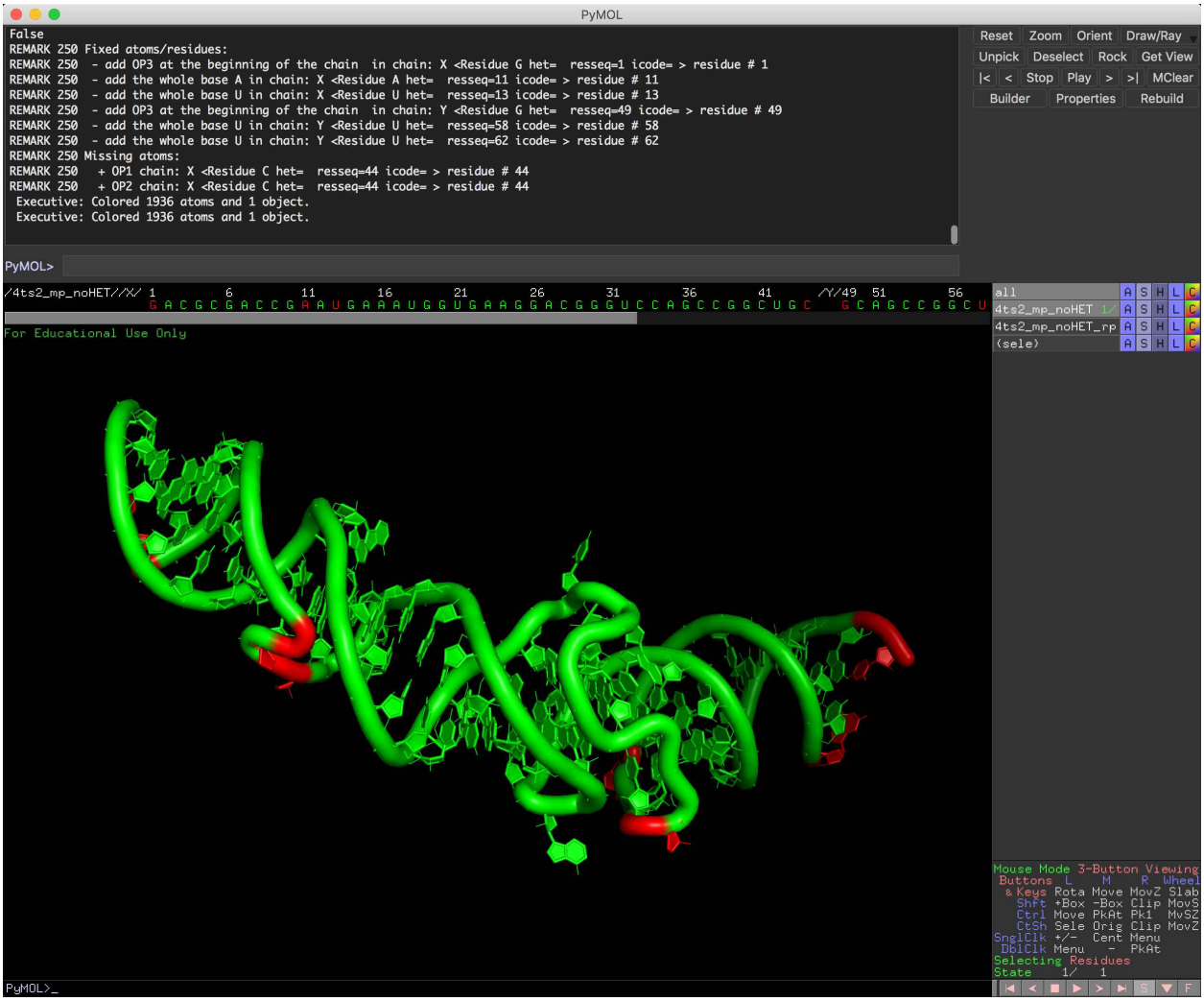
5.1 Inspect structure

There is new `--inspect` function for rna_pdb_tools.py that tells you what are missing atoms in your structure file.

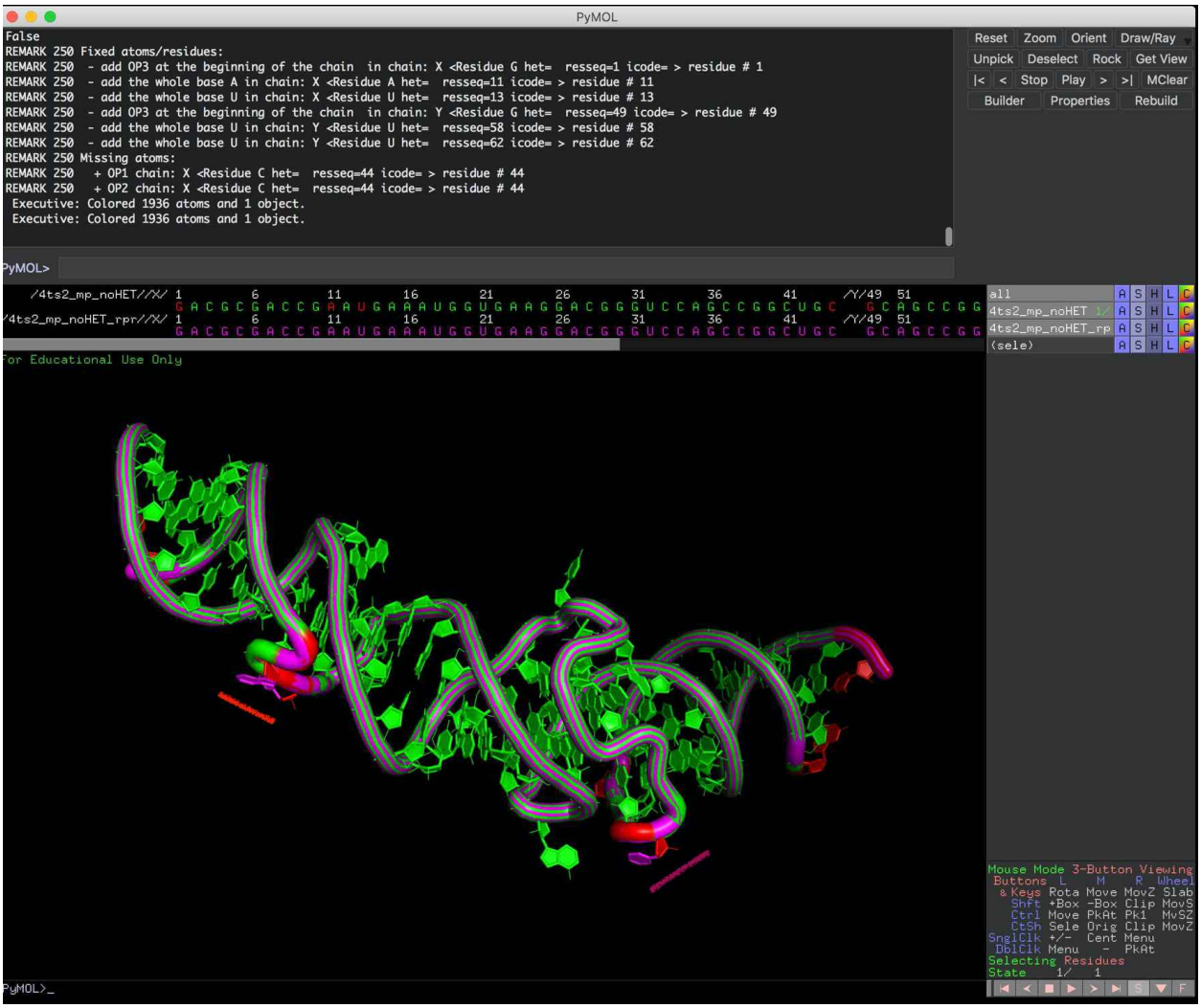
You can run it also from PyMOL, so in here you can see missing atoms directly in PyMOL (the object comes green and the residues missing atoms comes in red).

PyMOL:

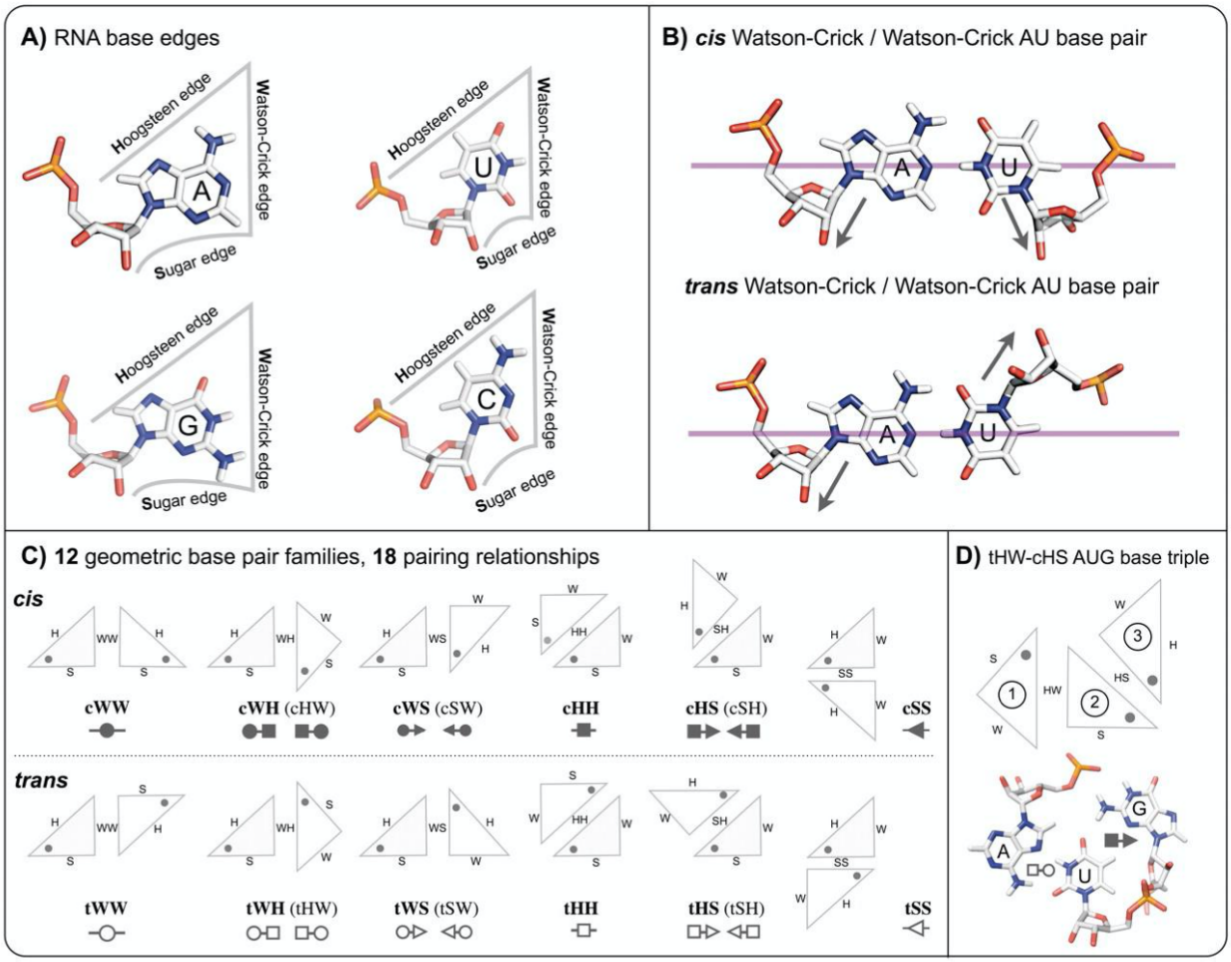
```
inspect <object name>
```



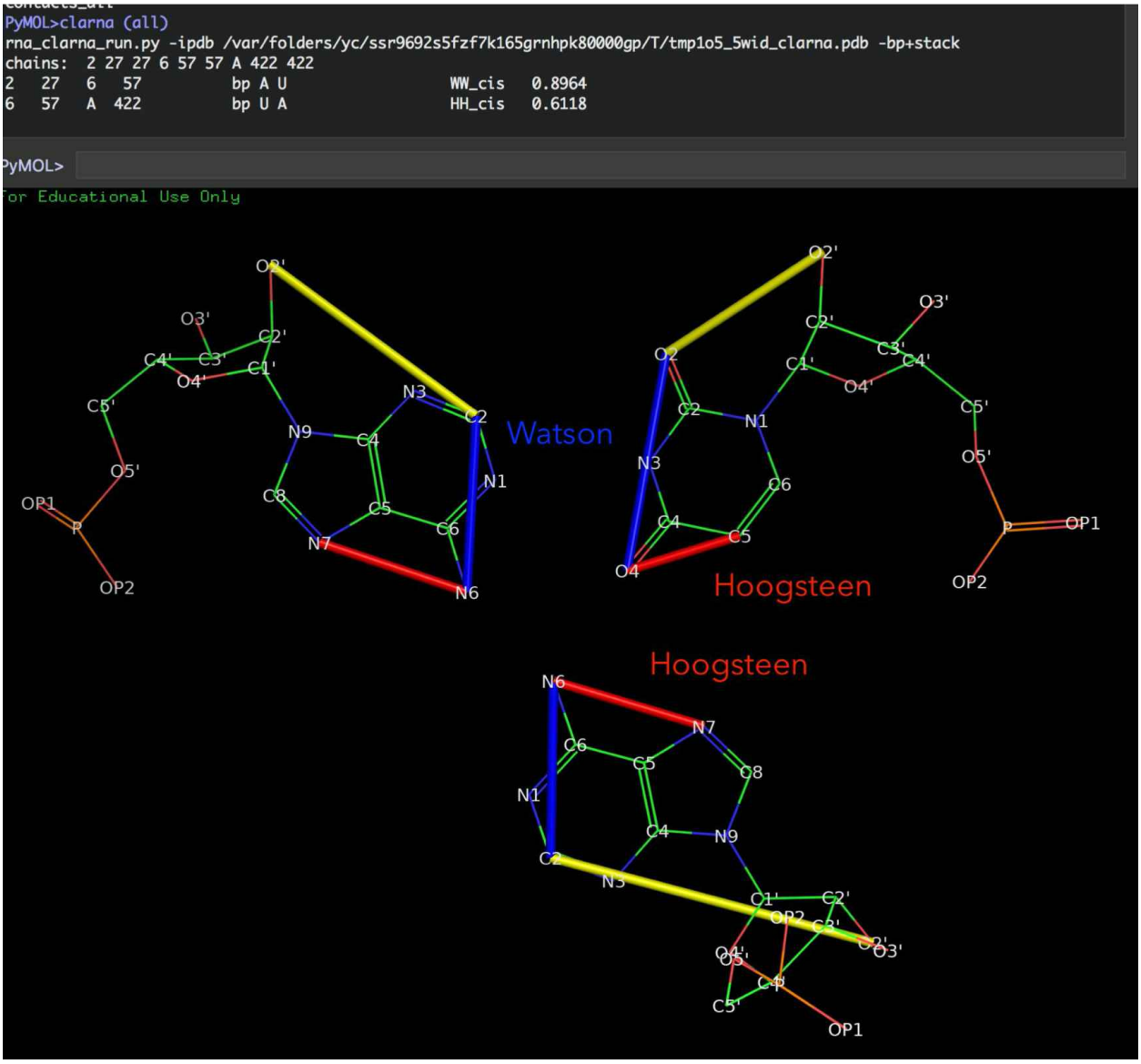
and here you can compare the input file vs file after `--rpr` (of rna_pdb_tools.py) to see what was rebuilt (in pink).


PyMOL
False
REMARK 250 Fixed atoms/residues:
REMARK 250 - add OP3 at the beginning of the chain in chain: X <Residue G het= resseq=1 icode= > residue # 1
REMARK 250 - add the whole base A in chain: X <Residue A het= resseq=11 icode= > residue # 11
REMARK 250 - add the whole base U in chain: X <Residue U het= resseq=13 icode= > residue # 13
REMARK 250 - add OP3 at the beginning of the chain in chain: Y <Residue G het= resseq=49 icode= > residue # 49
REMARK 250 - add the whole base U in chain: Y <Residue U het= resseq=58 icode= > residue # 58
REMARK 250 - add the whole base U in chain: Y <Residue U het= resseq=62 icode= > residue # 62
REMARK 250 Missing atoms:
REMARK 250 + OP1 chain: X <Residue C het= resseq=44 icode= > residue # 44
REMARK 250 + OP2 chain: X <Residue C het= resseq=44 icode= > residue # 44
Executive: Colored 1936 atoms and 1 object.
Executive: Colored 1936 atoms and 1 object.
Reset
Zoom
Orient
Draw/Ray
Unpick
Deselect
Rock
Get View
Stop
Play
MClear
Builder
Properties
Rebuild
PyMOL>
all
4ts2_mp_noHET
4ts2_mp_noHET_rp
(sele)
For Educational Use Only
Mouse Mode 3-Button Viewing
Selecting Residues
PyMOL>_

5.2 Show base pair edges



Leontis/Westhof classification of base pairings. (A) RNA bases - adenine (A), cytosine (C), guanine (G) and uracil (U) - involve one of three distinct edges: the Watson– Crick (W) edge, the Hoogsteen (H) edge, and the Sugar (S) edge. (B) Each pair of can interact in either cis or trans orientations with respect to the glycosidic bonds. (C) For these reasons, all base pairs can be grouped into twelve geometric base pair families and eighteen pairing relationships (bases are represented as triangles). Each pair is represented by a symbol that can be used in a secondary structure and a tertiary structure diagrams. Filled symbols mean cis base pair configuration, and open symbols, trans base pair. (D) Interestingly, bases can form triples and they have own classification devised by Leontis and coworkers (Creative Commons License) (A. S. Abu Almakarem, A. I. Petrov, J. Stombaugh, C. L. Zirbel, and N. B. Leontis, "Comprehensive survey and geometric classification of base triples in RNA structures.," Nucleic Acids Research, vol. 40, no. 4, pp. 1407–1423, Feb. 2012.)



Warning: This PyMOL function is very simple and works on standard atom naming, so to make sure that everything will work, get your structure in the RNA Puzzle ready format, See https://rna-tools.readthedocs.io/en/latest/main.html#get-rnapuzzle-ready

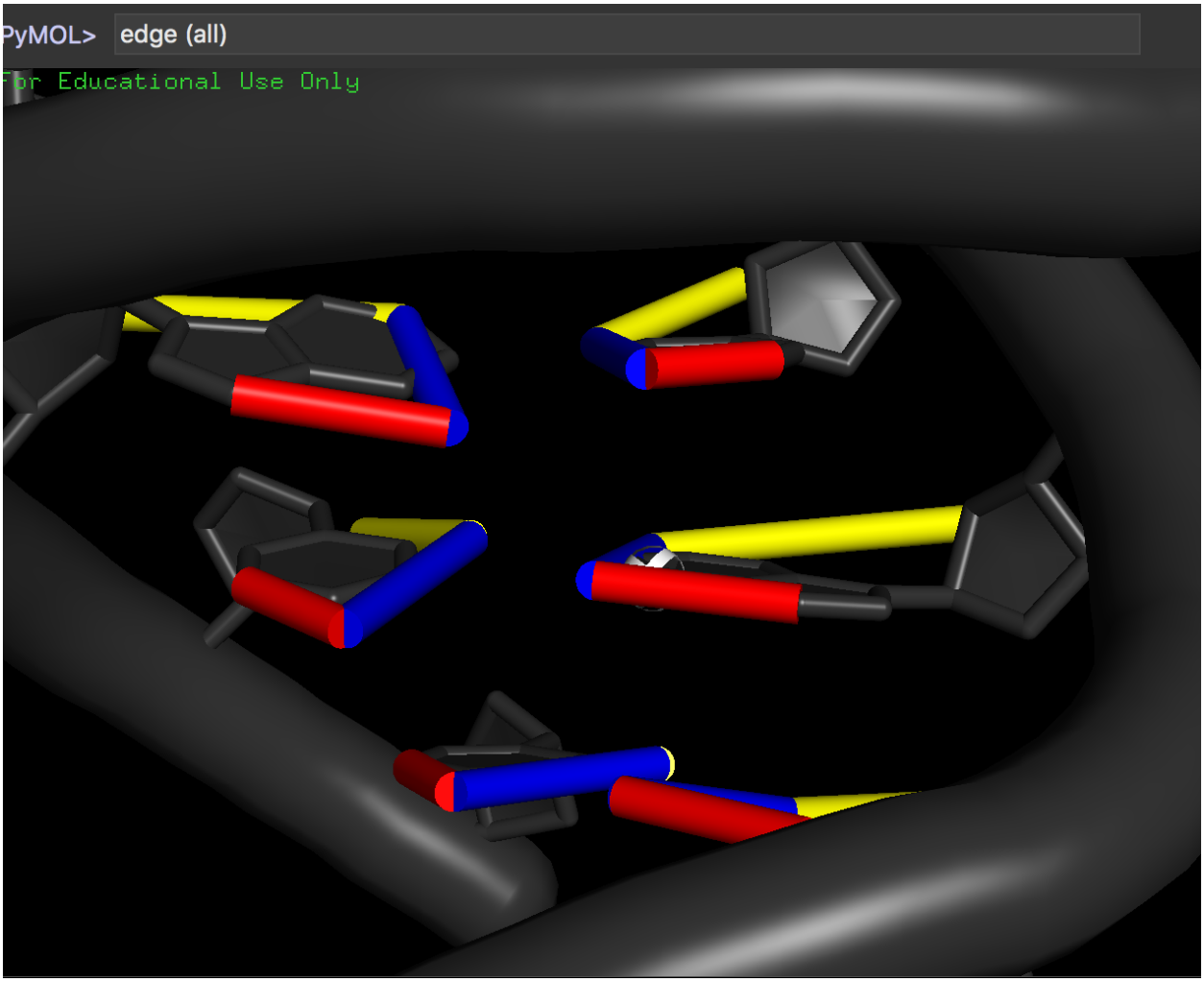
Type:

```
edges (<selection>)
```

e.g.,:

```
edges (all)
```

to show the edges drawn on bases.



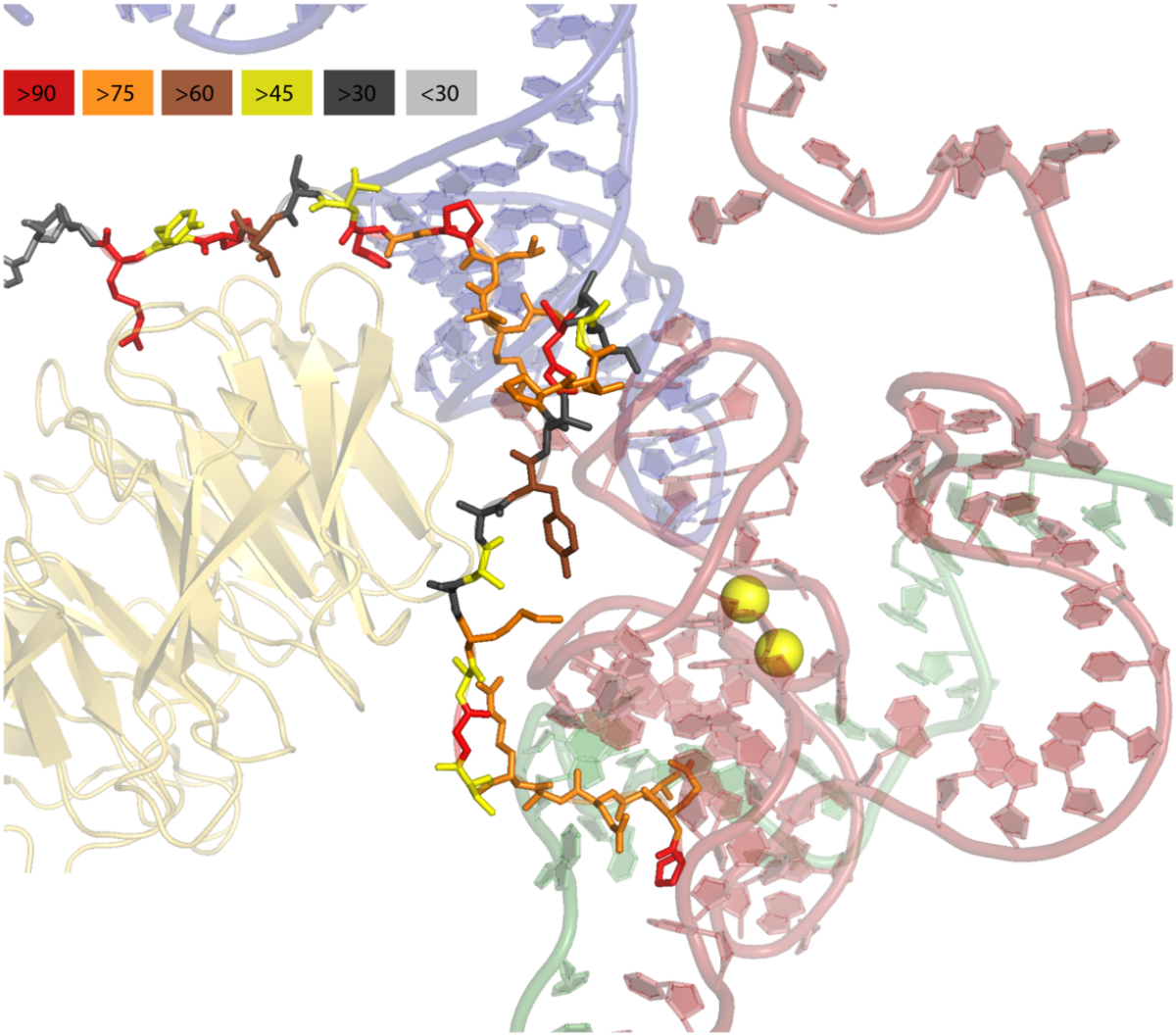
5.3 PyMOL4Spliceosome: all spliceosome structures in one PyMOL session

Download one PyMOL session with structures for each step.

See own project https://github.com/mmagnus/PyMOL4Spliceosome

5.4 PyMOL: Color by conservation

Show conserved regions of proteins in PyMOL.



See more: https://github.com/mmagnus/rna-tools/tree/master/rna_tools/tools/pymol_color_by_conserv

5.5 PyMOL Drawing

rna_tools.tools.pymol_drawing.pymol_drawing.**draw_circle**(*x*, *y*, *z*, *r=8.0*, *cr=1.0*, *cg=0.4*, *cb=0.8*, *w=2.0*)

Create a CGO circle

PARAMS

x, y, z
X, Y and Z coordinates of the origin

r
Radius of the circle

cr, cg, cb
Color triplet, [r,g,b] where r,g,b are all [0.0,1.0].

w
Line width of the circle

RETURNS
the CGO object (it also loads it into PyMOL, too).

rna_tools.tools.pymol_drawing.pymol_drawing.**draw_circle_selection**(*selName*, *r=None*, *cr=1.0*, *cg=0.4*, *cb=0.8*, *w=2.0*)

circleSelection – draws a cgo circle around a given selection or object

PARAMS

selName
Name of the thing to encircle.

r
Radius of circle. DEFAULT: This cript automatically defines the radius for you. If you select one atom and the resultant circle is too small, then you can override the script's calculation of r and specify your own.

cr, cg, cb
red, green and blue coloring, each a value in the range [0.0, 1.0]

RETURNS
The circle object.

rna_tools.tools.pymol_drawing.pymol_drawing.**draw_dist**(*54.729*, *28.9375*, *41.421*, *55.342*, *35.3605*, *42.745*)

https://sourceforge.net/p/pymol/mailman/message/25795427/

rna_tools.tools.pymol_drawing.pymol_drawing.**draw_dists**(*interactions*)

rna_tools.tools.pymol_drawing.pymol_drawing.**draw_vector**(*x1*, *y1*, *z1*, *x2*, *y2*, *z2*)

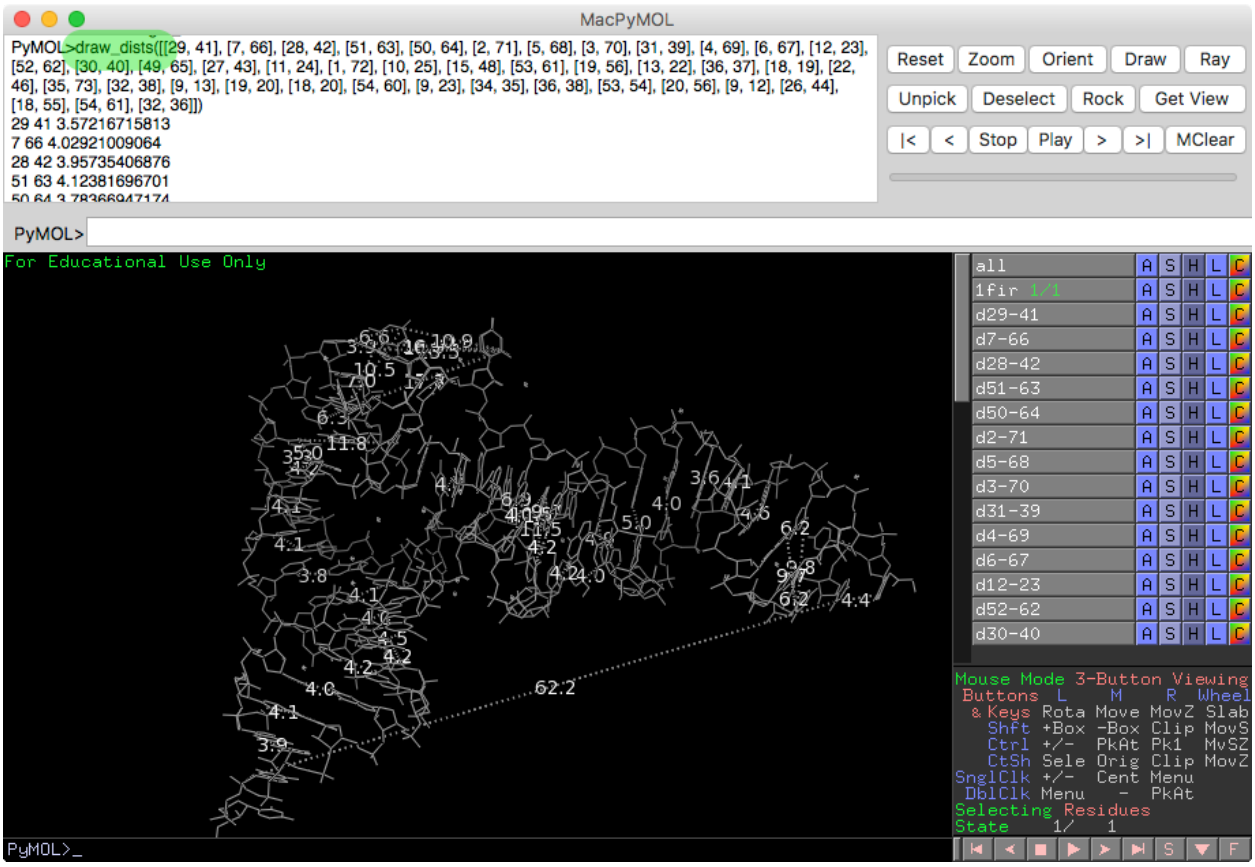
https://pymolwiki.org/index.php/CGOCylinder

Install PyMOL plugin to view the interactions with PyMOL:

```
run <path>rna-tools/tools/pymol_drawing/pymol_dists.py
```

and type:

```
draw_dists([[29, 41], [7, 66], [28, 42], [51, 63], [50, 64], [2, 71], [5, 68], [3, 70],␣
↪[31, 39], [4, 69], [6, 67], [12, 23], [52, 62], [30, 40], [49, 65], [27, 43], [11, 24],
↪ [1, 72], [10, 25], [15, 48], [53, 61], [19, 56], [13, 22], [36, 37], [18, 19], [22,␣
↪46], [35, 73], [32, 38], [9, 13], [19, 20], [18, 20], [54, 60], [9, 23], [34, 35], [36,
↪ 38], [53, 54], [20, 56], [9, 12], [26, 44], [18, 55], [54, 61], [32, 36]])
```



5.6 Install

After you install rna-tools, run these two lines your terminal:

```
$ echo "sys.path.append(``rna_tools_which.py --site`)" >> ~/.pymolrc
$ echo "PyMOL4RNA_PATH=``rna_tools_which.py`/tools/PyMOL4RNA/PyMOL4RNA.py'; cmd.
↪run(PyMOL4RNA_PATH)" >> ~/.pymolrc
```

so something like this will be added to your `~/.pymolrc`:

```
sys.path.append('/Users/magnus/work/src/rna-tools')
PyMOL4RNA_PATH='/Users/magnus/work/src/rna-tools/rna_tools/tools/PyMOL4RNA/PyMOL4RNA.py';
↪ cmd.run(PyMOL4RNA_PATH)
```

5.7 Libs: Pucker analysis

pucker.py is a PyMol script that returns the sugar pucker information (phase, amplitude, pucker) for a given selection.

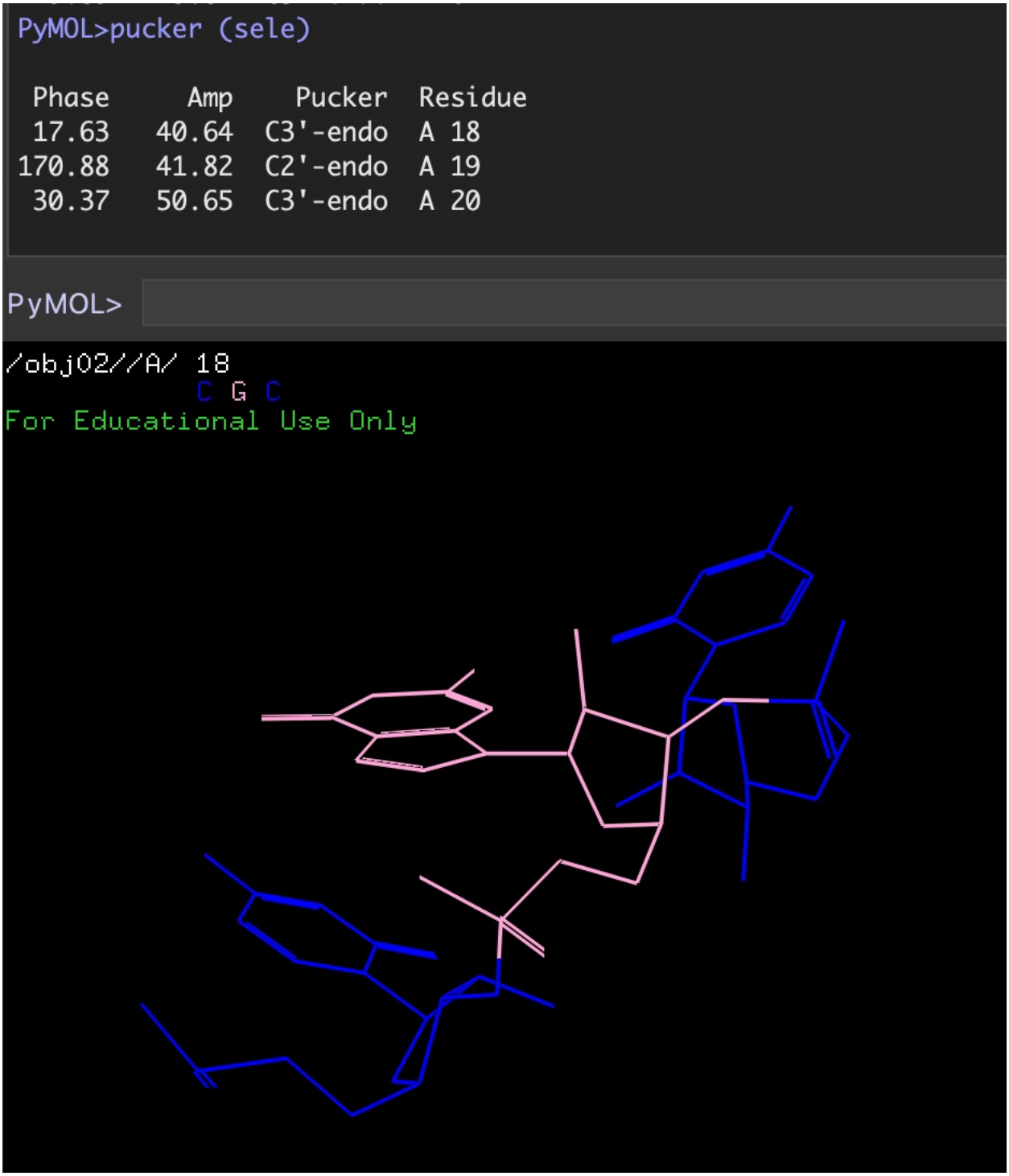
This script uses its own dihedral calculation scheme rather than the get_dihedral command. Thus, it is lightning fast!

If a selection does not contain any ribose sugars then an error message is returned.

Author: Sean Law (Institute: University of Michigan) adapted for Python 3 by magnus <mmagnus@fas.harvard.edu>.

Install, add *run <path>/rna-tools/rna_tools/tools/PyMOL4RNA/libs/pucker.py* to your ~/.pymolrc

Source: <https://pymolwiki.org/index.php/Pucker>


PyMOL>pucker (sele)
Phase Amp Pucker Residue
17.63 40.64 C3'-endo A 18
170.88 41.82 C2'-endo A 19
30.37 50.65 C3'-endo A 20
PyMOL>
/obj02//A/ 18
C G C
For Educational Use Only

CHAPTER

SIX

RNA-TOOLS & MAC/LINUX

6.1 PyMOL preview generator

https://github.com/mmagnus/rna-tools/tree/master/rna_tools/tools/pymol_preview_generator

Youtube video: https://www.youtube.com/watch?v=mNgW7sekgug

CHAPTER

SEVEN

RNA-TOOLS & JUPYTER NOTEBOOKS / COLAB

The tools collected here as rna-tools, ideally could be also used in IPython/Jupiter (https://ipython.org/notebook.html) Notebooks. We belive it would be valuable if we could, as scientists share our notebooks used for RNA structure analysis, e.g, protocols of modeling used in the RNA Puzzle challenge.

```
In [2]: seq = Seq.Seq("GGGUCAGGCCGGCGAAAGUCGCCACAGUUUGGGGAAAGCUGUGCAGCCUGUAACCCCCCCCACGAAAGUGGG")

In [3]: seq
Out[3]: GGGUCAGGCCGGCGAAAGUCGCCACAGUUUGGGGAAAGCUGUGCAGCCUGUAACCCCCCCCACGAAAGUGGG
```

Secondary structure prediction

```
In [12]: print seq.predict_ss()
         (((((((((.(((((...)))))(((((((.....)))))))...)))))..)))).(((((....)))))

In [13]: print seq.predict_ss(method='RNAsubopt')
         GGGUCAGGCCGGCGAAAGUCGCCACAGUUUGGGGAAAGCUGUGCAGCCUGUAACCCCCCCCACGAAAGUGGG  -3310    100
         (((((((((.((((.....)))))(((((((.....)))))))...)))))..)))).(((((....))))) -32.40
         (((((((((.(((((...)))))(((((((.....)))))))...)))))..)))).(((((....))))) -33.10
         (((((((((((((....))))).(((((((.....)))))))..)))))..)))).(((((....))))) -32.30

In [14]: print seq.predict_ss(method='ipknot')
         (((((((((((((....))))).(((((((.....)))))))..)))))..)))).(((((....)))))

In [15]: print seq.predict_ss(method='centroid_fold')
         (((((((((.(((....)))).(((((((.....)))))))..)))))..)))).(((((....))))) (g=1,th=0.5,e=-27.26)

In [16]: print seq.predict_ss(method='contextfold')
         (((.((((((((((....)))).(((((((.......)))))))..)))))...))).(((((....)))))
```

See more at https://github.com/mmagnus/rna-tools/blob/master/rp18.ipynb https://github.com/mmagnus/rna-tools/blob/master/rp19.ipynb

7.1 Share your notebooks

You can share Jupyter notebooks from your Google Drive using the new Jupyter Drive. This allows you share Jupyter notebooks like NBViewr with all the access control that Google Drive provides. You can also push your notebooks to a Github repository, so then can be rendered for easy viewing.

E.g., https://github.com/mmagnus/rna-tools/blob/master/rp18.ipynb

7.2 Use Colab

Some of the functions of rna-tools will work also on Colab.

E.g., ClaRNA https://colab.research.google.com/drive/1rcPz7ZLWpn-hbfJo8hpz6ZuMGiGGmKeW

7.3 Learn Jupyter

This is a quick introduction to jupyter which is the IPython version 3. It covers some of the new and interesting features about Jupyter.

https://www.youtube.com/watch?v=Rc4JQWowG5I

CHAPTER

EIGHT

RNA-TOOLS & EMACS

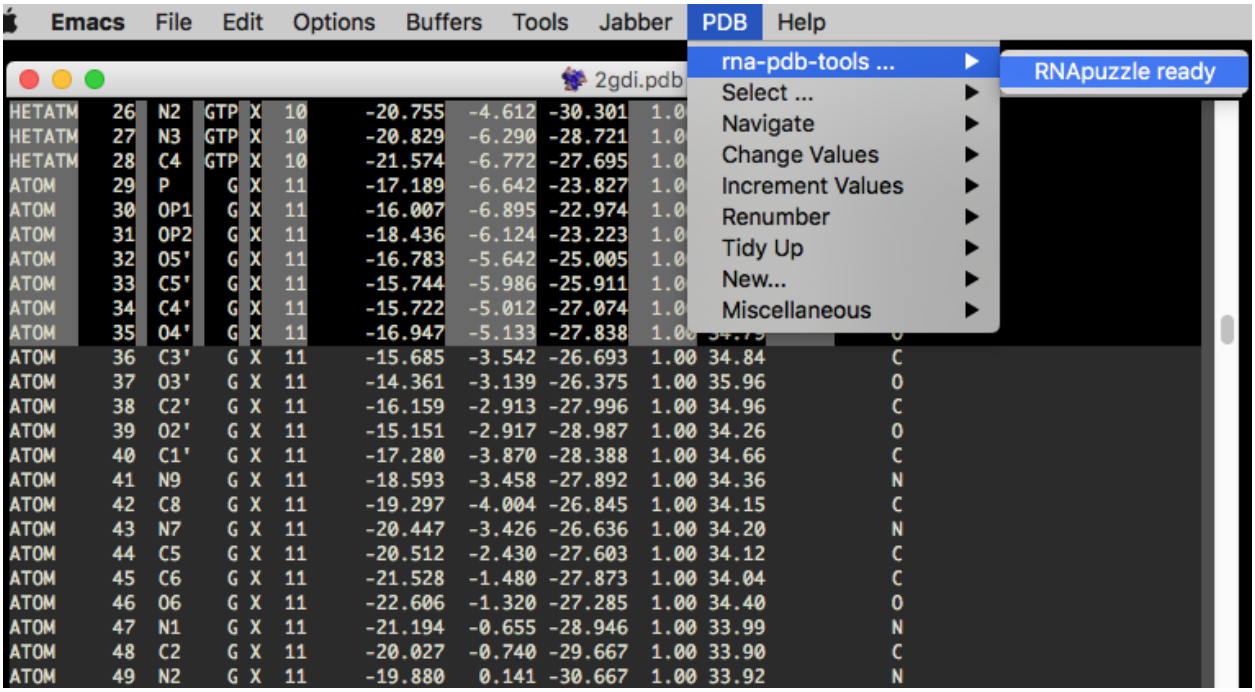
Warning: Proof of concept

rna-tools can be used side-by-side https://github.com/mmagnus/emacs-pdb-mode to edit files structural files in the PDB format.

Emacs /imæks/ and its derivatives are a family of text editors that are characterized by their extensibility.[2] The manual for the most widely used variant, GNU Emacs, describes it as "the extensible, customizable, self-documenting, real-time display editor". Development of the first Emacs began in the mid-1970s and continues actively as of 2017. (https://en.wikipedia.org/wiki/Emacs)

pdb-mode (https://github.com/mmagnus/emacs-pdb-mode not authored by me, I'm a maintainer, and a beginner developer) is an emacs-lisp minor mode for Emacs to perform a number of useful editing functions on Protein DataBank (PDB) formatted files. XEmacs and/or GNU Emacs are available for most computing platforms.

Youtube video: https://www.youtube.com/embed/o99YFbLSVRw



CHAPTER

NINE

RNA-TOOLS & GEEKBOOK

Warning: Proof of concept

G33KB00K - eXtreme eXtendable note taking system for nerds/geeks (including scientists!) (= beautiful html generator of your markdown-based notes) docs: http://geekbook.rtfd.io

Marcin Magnus (mmagnus) & Pietro Boccaletto (akaped)

The code of the project can be found at GitHub (https://github.com/mmagnus/geekbook).

A neat way how to combine Emacs/Atom/Sublime editor + Markdown Syntax + Git + Html engine (bootstrap/python) to get the best notes-talking experience ever. Highly customizable with plugins written in Python. What's the most important, under the hood it's just a set of Markdown files.. you can do with them whatever you want, e.g. you can Pandoc (http://pandoc.org/epub.html) them to epub (that's origin of "book" part of the name).

9.1 Draw VARNA-based image of RNA secondary structure

Type:

```
<pre>[ss:rna]
UUUCUGUAUAAUGCCGAUAAUAAGGUUCGGCAGUUUCUACCAAACAGCCGUAAACUGUUUGACUACAGUAA
((.(((((...((((((.........))))))........(((((((.......)))))))..)))))))
</pre>
```

Warning: Keep exactly the same syntax as in the example above and below.

The syntax:

```
<pre>
[ss:/name of your seq/]
/seq/
/ss/
</pre>
# ^ not <pre/> nor <pre>. Keep a new line after this syntax. So don't do:
</pre>
<pre>

but
```

(continues on next page)

(continued from previous page)

```
</pre>

<pre>
# ^ this could be fixed at some point
```

Warning: This plugin will change your Markdown file, so make sure that your editor will detect this change and ask you to reload the file!

to get a VARNA-drawn image of secondary structure.

CHAPTER

TEN

RNA PUZZLE SUBMISSION

The RNA Puzzle organizers required ONE file with your submissions in the NMR-style multiple model PDB format.

First, prepare your structures in the folder and run to get them RNApuzzle ready (*_rpr*):

```
$ for i in *.pdb; do rna_pdb_tools.py --get-rnapuzzle-ready $i > ${i/.pdb/_rpr.pdb}; done
```

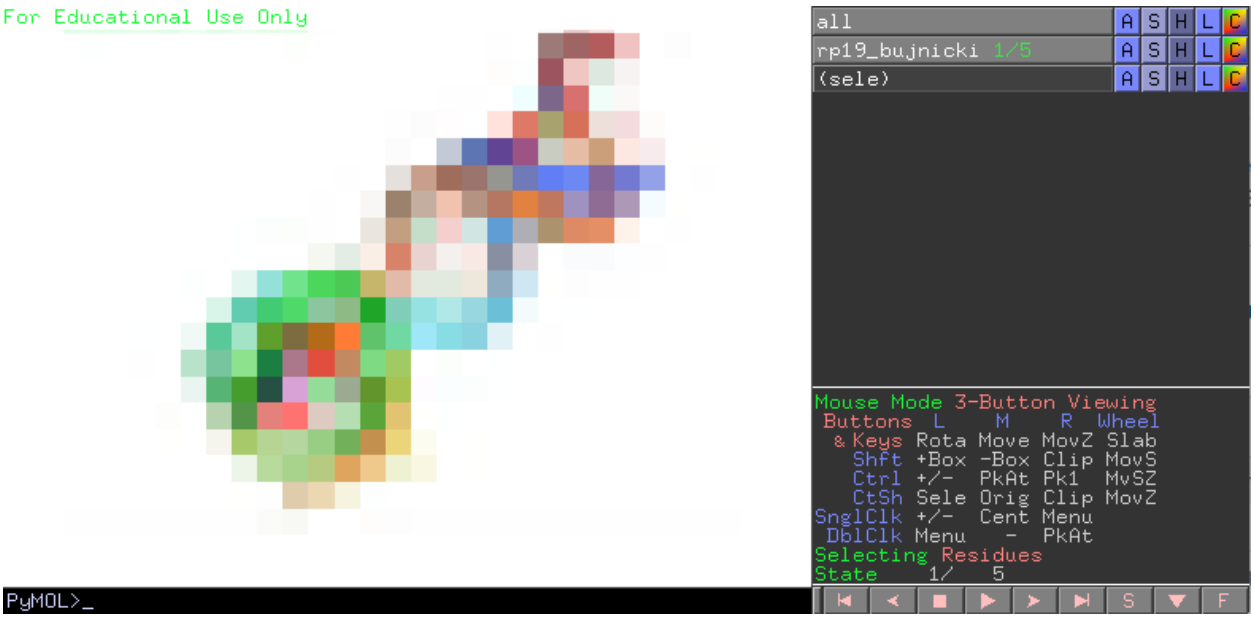
merge them as one file in the order as you like (or use *):

```
$ rna_pdb_merge_into_one.py 02_19pz_v1_SimRNA3.22_thrs6.60A_clust02-000001_AA_out_rpr.
↪pdb \
09_19pz_v2_SimRNA3.22_thrs6.60A_clust03-000001_AA_out_rpr.pdb \
d311d821-a075-4df0-bd7d-1dcf7669dad9_ALL_thrs6.20A_clust01-000001_AA_out_rpr.pdb \
d311d821-a075-4df0-bd7d-1dcf7669dad9_ALL_thrs6.20A_clust03-000001_AA_out_rpr.pdb \
05_19pz_v1_SimRNA4.xx_thrs6.60A_clust02-000001_AA_out_rpr.pdb  > rp19_bujnicki.pdb
```

and verify your file with the template provided by the organizers (if provided)::

```
$ diffpdb --method diff Reference_19.pdb rp19_bujnicki.pdb
#<empty = no difference but xyz columns, OK!>
```

diffpdb is a part of the rna-tools package.



In terminal:

```
$ head -n 5 Reference_19.pdb rp19_bujnicki.pdb
==> Reference_19.pdb <==
MODEL        1
ATOM      1  P     G A   1       0.000   0.000   0.000  1.00  0.00           P
ATOM      2  OP1   G A   1       0.000   0.000   0.000  1.00  0.00           O
ATOM      3  OP2   G A   1       0.000   0.000   0.000  1.00  0.00           O
ATOM      4  O5'   G A   1       0.000   0.000   0.000  1.00  0.00           O
==> rp19_bujnicki.pdb <==
MODEL        1
ATOM      1  P     G A   1      31.463  14.180  -0.676  1.00  0.00           P
ATOM      2  OP1   G A   1      31.412  12.806  -1.223  1.00  0.00           O
ATOM      3  OP2   G A   1      30.646  15.083  -1.517  1.00  0.00           O
ATOM      4  O5'   G A   1      30.955  14.212   0.842  1.00  0.00           O

$ tail -n 5 Reference_19.pdb rp19_bujnicki.pdb
==> Reference_19.pdb <==
ATOM   1325  C5    C B  22       0.000   0.000   0.000  1.00  0.00           C
ATOM   1326  C6    C B  22       0.000   0.000   0.000  1.00  0.00           C
TER    1327        C B  22
ENDMDL
END
==> rp19_bujnicki.pdb <==
ATOM   1325  C5    C B  22      29.927  21.506  -6.542  1.00  0.00           C
ATOM   1326  C6    C B  22      29.822  22.338  -5.500  1.00  0.00           C
TER    1327        C B  22
ENDMDL
END
```

The Bujnicki lab is using this script to process the results and send the results, you can hack it for your own case:

```
[mm] rnapuzzle_sender$ git:(master)  ./rnapuzzle_sender.py
rnapuzzle_sender

Usage: rnapuzzle_sender.py

Options:
  -h, --help            show this help message and exit
  -d DIR, --dir=DIR
  -s EMAIL_SUBJECT, --email_subject=EMAIL_SUBJECT
                        email subject
```

File: *rna-tools/rna_tools/tools/rnapuzzle_sender*.

CHAPTER

ELEVEN

SELECTION

These functions are intended to be imported to tools to give a unified framework for making selections.

rna_tools.tools.extra_functions.select_fragment.**select_pdb_fragment**(*txt*, *separator='-'*, *splitting='[:\\+]'*, *verbose=False*)

Take txt such as `A:1-31+B:1-11` and parse into:

```
OrderedDict([('A', [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14,
15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31]),
('B', [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11])])
```

> **Warning:** e.g. for A:1-31, resi 31 is included

rna_tools.tools.extra_functions.select_fragment.**select_pdb_fragment_pymol_style**(*txt*)

Take txt such as A/10-15/P and parse into:

```
A/57/O2' -> ['A', ['57'], "O2'"]
```

If you want to combine a few subselections, please use `,`:

```
--model_ignore_selection "A/57/O2',A/58/O2'"
```

> **Warning:** e.g. for A:1-31, resi 31 is included

CHAPTER

TWELVE

TIPS

12.1 Run in batch

You can easily run a single tool in batch and rename new files:

```
$ for i in *.pdb; do rna_pdb_tools.py --get_rnapuzzle_ready $i > ${i/.pdb/_rpr.pdb}; done
```

or write new files in a different folder (*out*):

```
$ for i in *.pdb; do rna_pdb_tools.py --get_rnapuzzle_ready $i > ../out/$i; done
```

You can also easily run a single tool parallel using **parallel_**:

```
$ parallel "rna_add_chain.py -c A {} > ../nchain/{}" ::: *.pdb
# ex2
$ parallel "rna_clashscore.py {} > {}.csv" ::: *.pdb
```

12.2 Using sed

sed (stream editor) is a Unix utility that parses and transforms text, using a simple, compact programming language.

You can used sed to find & replace parts of text files:

```
$ head 1msy_rnakbmd_decoy1661_clx.pdb.outCR
Classifier: Clarna
chains:  1 27
     2       26          bp G U                  WW_cis   0.8500
     3       25          bp C G                  WW_cis   0.8114
     4       24          bp U A                  WW_cis   0.9222
     5       23          bp C G                  WW_cis   0.9038
     6       22          bp C G                  WW_cis   0.8913
     9       10          bp G U                  SH_cis   0.8563
    10       19          bp U A                 WH_tran   0.7826
    11       18          bp A G                 HS_tran   0.7620

$ sed 's/chains: /chains: A/' 1msy_rnakbmd_decoy1661_clx.pdb.outCR
Classifier: Clarna
chains: A 1 27
     2       26          bp G U                  WW_cis   0.8500
```

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```
    3       25          bp C G                  WW_cis   0.8114
    4       24          bp U A                  WW_cis   0.9222
    5       23          bp C G                  WW_cis   0.9038
    6       22          bp C G                  WW_cis   0.8913
    9       10          bp G U                  SH_cis   0.8563
   10       19          bp U A                 WH_tran   0.7826
   11       18          bp A G                 HS_tran   0.7620
   12       17          bp C G                  WW_cis   0.7242
```

Read more about sed.

12.3 In PyMOL

Quickref:

```
set ignore_case, off
```

Rename a chain:

```
PyMOL>alter (sele), chain="B"
Alter: modified 708 atoms.
PyMOL>sort
```

don't forget about *sort*.

To select all, use *PyMOL>alter all, resv -= 12*.

To renumber a fragment starting with 24 to 29, select the fragment and:

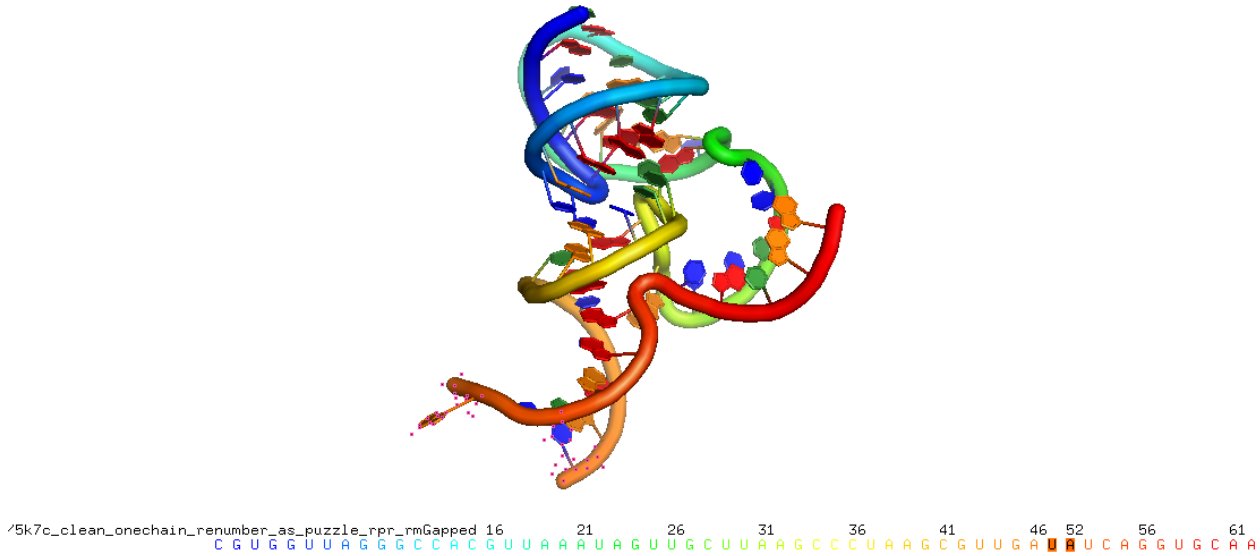
```
PyMOL>alter (sele), resv += 5
 Alter: modified 109 atoms.
```

To renumber residues:

```
PyMOL>alter (chain B), resv -= 44
Alter: modified 708 atoms.
PyMOL>sort
```

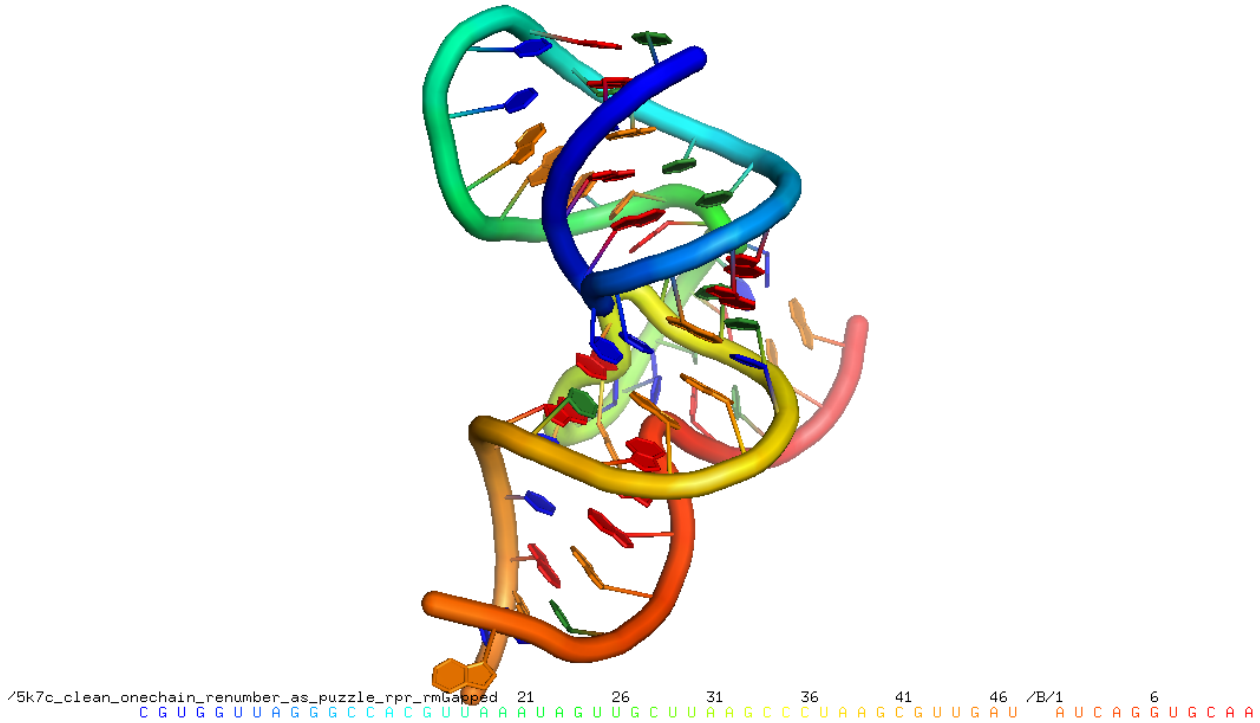
Read more.

The example of the pistol ribozyme editing.



Run:

```
PyMOL>alter (sele), chain="B"
 Alter: modified 236 atoms.
PyMOL>alter (chain B), resv -= 51
 Alter: modified 236 atoms.
PyMOL>sort
```



12.4 In Python

To get residue index use:

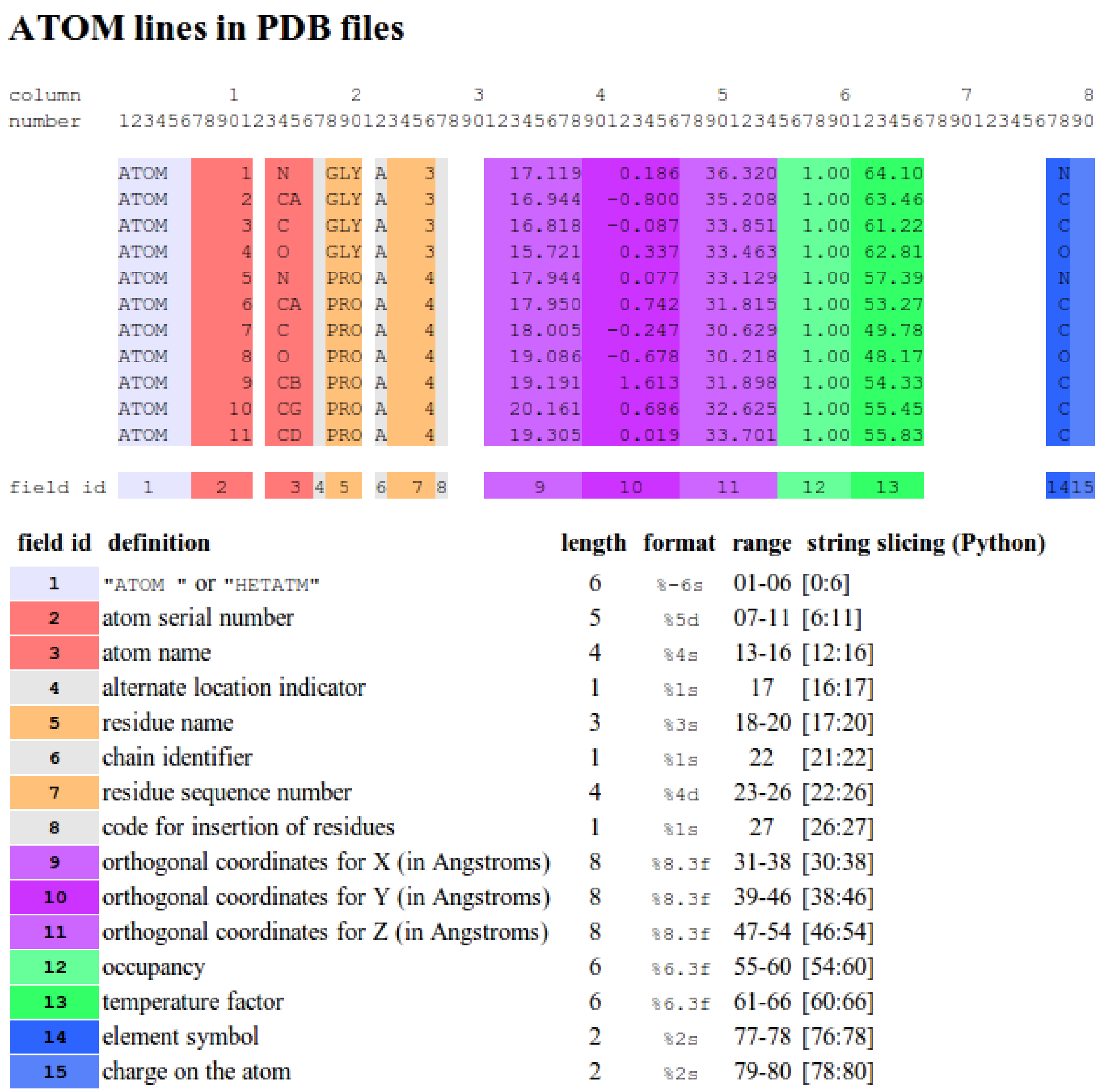
```
resi = int(l[22:26].strip())
```

Example:

```
ATOM      1  P     C A   1     -16.936  -3.789  68.770  1.00 11.89           P
```

Qucikref:

```
COLUMNS PYTHON     DATA  TYPE    FIELD        DEFINITION
-------------------------------------------------------------------------------
 1 -  6 [0:6]      Record name   "ATOM  "
 7 - 11 [6:11]     Integer       serial       Atom  serial number.
13 - 16 [12:16]    Atom          name         Atom name.
17      [16]       Character     altLoc       Alternate location indicator.
18 - 20 [17:20]    Residue name  resName      Residue name.
22      [21]       Character     chainID      Chain identifier.
23 - 26 [22:26]    Integer       resSeq       Residue sequence number.
27      [26]       AChar         iCode        Code for insertion of residues.
31 - 38 [30:38]    Real(8.3)     x            Orthogonal coordinates for X in Angstroms.
39 - 46 [38:46]    Real(8.3)     y            Orthogonal coordinates for Y in Angstroms.
47 - 54 [46:54]    Real(8.3)     z            Orthogonal coordinates for Z in Angstroms.
55 - 60 [54:60]    Real(6.2)     occupancy    Occupancy.
61 - 66 [60:66]    Real(6.2)     tempFactor   Temperature  factor.
77 - 78 [76:78]    LString(2)    element      Element symbol, right-justified. # l[76:78]
79 - 80 [78:80]    LString(2)    charge       Charge  on the atom.
```



ATOM lines in PDB files

```
column           1         2         3         4         5         6         7         8
number  12345678901234567890123456789012345678901234567890123456789012345678901234567890

        ATOM      1  N   GLY A   3      17.119   0.186  36.320  1.00 64.10           N
        ATOM      2  CA  GLY A   3      16.944  -0.800  35.208  1.00 63.46           C
        ATOM      3  C   GLY A   3      16.818  -0.087  33.851  1.00 61.22           C
        ATOM      4  O   GLY A   3      15.721   0.337  33.463  1.00 62.81           O
        ATOM      5  N   PRO A   4      17.944   0.077  33.129  1.00 57.39           N
        ATOM      6  CA  PRO A   4      17.950   0.742  31.815  1.00 53.27           C
        ATOM      7  C   PRO A   4      18.005  -0.247  30.629  1.00 49.78           C
        ATOM      8  O   PRO A   4      19.086  -0.678  30.218  1.00 48.17           O
        ATOM      9  CB  PRO A   4      19.191   1.613  31.898  1.00 54.33           C
        ATOM     10  CG  PRO A   4      20.161   0.686  32.625  1.00 55.45           C
        ATOM     11  CD  PRO A   4      19.305   0.019  33.701  1.00 55.83           C

field id  1    2     3 4 5  6  7 8     9       10      11      12    13             1415
```

field id	definition	length	format	range	string slicing (Python)
1	"ATOM " or "HETATM"	6	%-6s	01-06	[0:6]
2	atom serial number	5	%5d	07-11	[6:11]
3	atom name	4	%4s	13-16	[12:16]
4	alternate location indicator	1	%1s	17	[16:17]
5	residue name	3	%3s	18-20	[17:20]
6	chain identifier	1	%1s	22	[21:22]
7	residue sequence number	4	%4d	23-26	[22:26]
8	code for insertion of residues	1	%1s	27	[26:27]
9	orthogonal coordinates for X (in Angstroms)	8	%8.3f	31-38	[30:38]
10	orthogonal coordinates for Y (in Angstroms)	8	%8.3f	39-46	[38:46]
11	orthogonal coordinates for Z (in Angstroms)	8	%8.3f	47-54	[46:54]
12	occupancy	6	%6.3f	55-60	[54:60]
13	temperature factor	6	%6.3f	61-66	[60:66]
14	element symbol	2	%2s	77-78	[76:78]
15	charge on the atom	2	%2s	79-80	[78:80]

(source: http://cupnet.net/pdb-file-atom-line-memo/)

12.5 Working with cluster

Tips:

```
# get your pdb files
[mm] ade rsync -v peyote2:'~/ade/*.pdb' . # ' is required!
```

See long name with `qstat`:

```
magnus@peyote2:~$ qstat -xml | tr '\n' ' ' | sed 's#<job_list[^>]*>#\n#g' \
>   | sed 's#<[^>]*>##g' | grep " " | column -t
4752204  5.54737  r_6bd26658_run_04                magnus  dr  2017-02-20T22:09:04  all.
↪q@c6.cluster3.genesilico.pl   10
4752201  5.54737  r_6bd26658_run_01                magnus  dr  2017-02-20T22:09:04  all.
↪q@c6.cluster3.genesilico.pl   10
4752203  5.54737  r_6bd26658_run_03                magnus  dr  2017-02-20T22:09:04  all.
↪q@c6.cluster3.genesilico.pl   10
4752202  5.54737  r_6bd26658_run_02                magnus  dr  2017-02-20T22:09:04  all.
↪q@c6.cluster3.genesilico.pl   10
4805710  5.54737  r_hTERC_251-451-85d4ac69_run_01  magnus  r   2017-08-20T17:04:15  all.
↪q@c11.cluster3.genesilico.pl  10
4805711  5.54737  r_hTERC_251-451-85d4ac69_run_02  magnus  r   2017-08-20T17:04:15  all.
↪q@c11.cluster3.genesilico.pl  10
4805712  5.54737  r_hTERC_251-451-85d4ac69_run_03  magnus  r   2017-08-20T17:04:15  all.
↪q@c8.cluster3.genesilico.pl   10
4805713  5.54737  r_hTERC_251-451-85d4ac69_run_04  magnus  r   2017-08-20T17:04:15  all.
↪q@c8.cluster3.genesilico.pl   10
4805714  5.54737  r_hTERC_251-451-85d4ac69_run_05  magnus  r   2017-08-20T17:04:15  all.
↪q@c8.cluster3.genesilico.pl   10
4805715  5.54737  r_hTERC_251-451-85d4ac69_run_06  magnus  r   2017-08-20T17:04:15  all.
↪q@c8.cluster3.genesilico.pl   10
4805716  5.54737  r_hTERC_251-451-85d4ac69_run_07  magnus  r   2017-08-20T17:04:15  all.
↪q@c8.cluster3.genesilico.pl   10
4805728  5.54737  r_mCherry_sub3-3c970489_run_03   magnus  r   2017-08-20T17:21:15  all.
↪q@c15.cluster3.genesilico.pl  10
```

https://stackoverflow.com/questions/26104116/qstat-and-long-job-names

12.6 Numbering line used in my flat-file notes

Numbering:

```
|1.......|10.......|20.......|30.......|40.......|50.......|60.......|70.......|80.......
↪|90.......
12345678911234567892123456789312345678941234567895123456789612345678971234567898123456789912345678
```

12.7 TER format

Example of pro TER:

```
ATOM   72307  C4    U x   9     304.768 147.960 320.897  1.00218.84           C
ATOM   72308  O4    U x   9     304.171 146.902 321.104  1.00225.09           O
ATOM   72309  C5    U x   9     304.190 149.269 320.912  1.00211.91           C
ATOM   72310  C6    U x   9     304.960 150.336 320.668  1.00205.76           C
TER    72311        U x   9
```

12.8 Add missing atoms

Add missing atoms etc.:

```
(py37) [mx] cwc46$ pdbfixer prp46.pdb --add-atoms all --add-residues
```

Read more:

- https://github.com/openmm/pdbfixer
- http://htmlpreview.github.io/?https://raw.github.com/pandegroup/pdbfixer/master/Manual.html

12.9 Test for Cuda

Run a test for CUDA:

```
rna_test_cuda.py
> rna_test_cuda.py:9 in <module>- torch.cuda.current_device(): 0
> rna_test_cuda.py:10 in <module>
  torch.cuda.device(0): <torch.cuda.device object at 0x146bf9bf7b80>
> rna_test_cuda.py:11 in <module>- torch.cuda.is_available(): True
Using device: cuda

NVIDIA A40
Memory Usage:
Allocated: 0.0 GB
Reserved:  0.0 GB

tensor([[ 0.9374,  1.1526, -0.5648,  0.9870]], device='cuda:0')
```

CHAPTER

THIRTEEN

EXAMPLES OF WORKFLOWS

13.1 Example #1

The native:

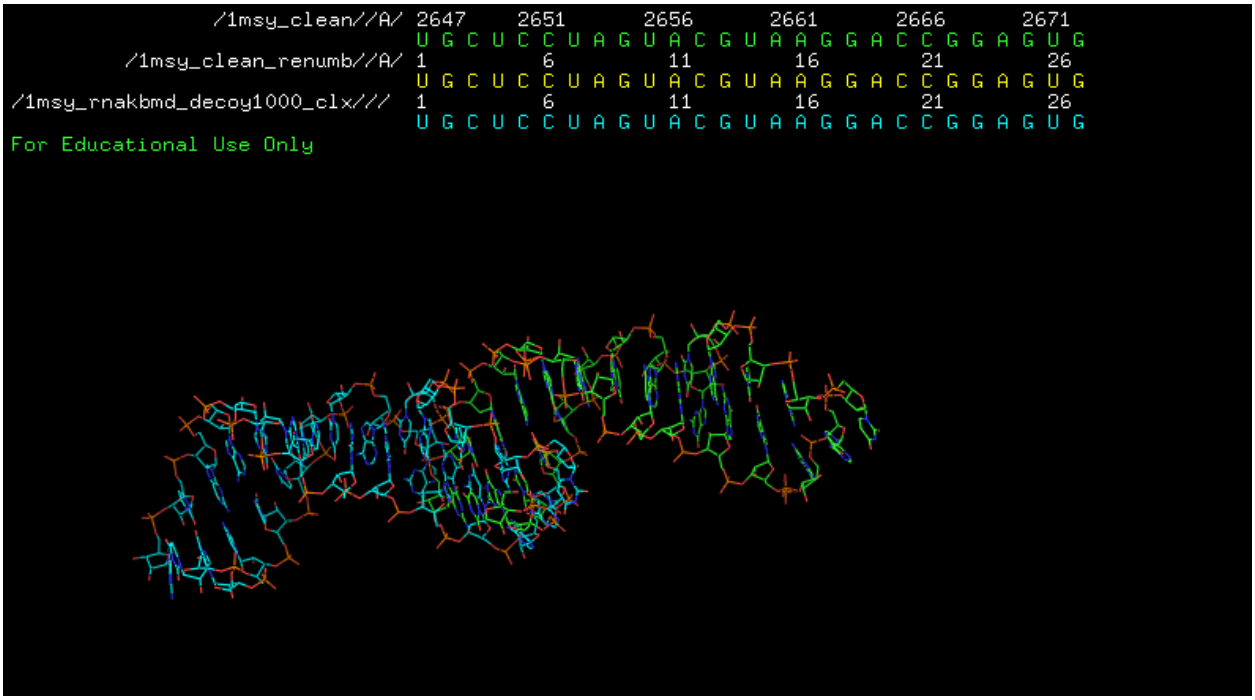
```
[mq] md_1msy_clx$ cat 1msy_clean.pdb.outCR
Classifier: Clarna
chains:  A 2647 2673
A 2648   A 2672          bp G U                  WW_cis   0.8732
A 2649   A 2671          bp C G                  WW_cis   0.9160
A 2650   A 2670          bp U A                  WW_cis   0.9289
A 2651   A 2669          bp C G                  WW_cis   0.9439
A 2652   A 2668          bp C G                  WW_cis   0.9281
A 2655   A 2656          bp G U                  SH_cis   0.9227
A 2656   A 2665          bp U A                 WH_tran   0.8526
A 2657   A 2664          bp A G                 HS_tran   0.8513
A 2658   A 2663          bp C G                  WW_cis   0.9421
A 2659   A 2662          bp G A                 SH_tran   0.7619
```

but analyzed structres are like:

```
[mq] md_1msy_clx$ cat struc/1msy_rnakbmd_decoy1478_clx.pdb.outCR
Classifier: Clarna
chains: A 1 27
 2       26          bp G U                  WW_cis   0.7196
 3       25          bp C G                  WW_cis   0.6702
 4       24          bp U A                  WW_cis   0.8911
 5       23          bp C G                  WW_cis   0.8925
 6       22          bp C G                  WW_cis   0.9026
 9       10          bp G U                  SH_cis   0.8714
 10       19          bp U A                 WH_tran   0.7279
 11       18          bp A G                 HS_tran   0.8810
 12       17          bp C G                  WW_cis   0.9115
```

You have to renumber 1msy_clean.pdb to 1:27:

```
$ rna_pdb_tools.py --edit 'A:2647-2673>A:1:17' 1msy_clean.pdb > 1msy_clean_renumb.pdb
```



13.2 Example #2

Listing:

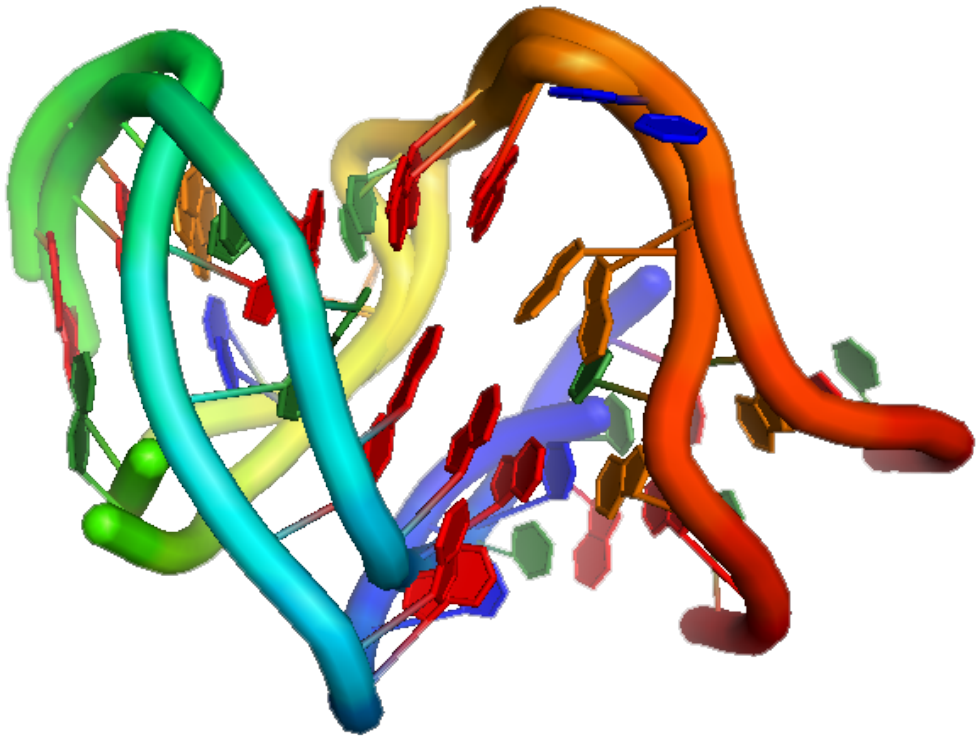
```
$ rna_pdb_tools.py --get-seq 1nuj_rnakbmd_decoy1000_clx.pdb
> 1nuj_rnakbmd_decoy1000_clx.pdb A:1-13
CGGACCGAGCCAG
> 1nuj_rnakbmd_decoy1000_clx.pdb B:14-24
GCUGGGAGUCC

$ rna_pdb_tools.py --get-seq 1nuj_clean.pdb
> 1nuj_clean.pdb A:18-30
CGGACCGAGCCAG
> 1nuj_clean.pdb B:39-49
GCUGGGAGUCC

$ rna_pdb_tools.py --edit 'A:18-30>A:1-13,B:39-49>B:14-24' 1nuj_clean.pdb > 1nuj_clean_
↪renumber.pdb

$ rna_pdb_tools.py --get-seq 1nuj_clean_renumber.pdb
> 1nuj_clean_renumber.pdb A:1-13
CGGACCGAGCCAG
> 1nuj_clean_renumber.pdb B:14-24
GCUGGGAGUCC
```

13.3 Example #3

Starting structure doesn't have chain id:

```
# add chain A
$ parallel "rna_add_chain.py -c A {} > ../struc_with_chain/{}" ::: *.pdb
# edit the second part of the new chain A as B
$ parallel "rna_pdb_gtools.py --edit 'A:14-27>B:14-27' {} > out/{}" ::: *.pdb
```

```
/1duq_rnakbnm_decoy0473_amb_clx//A/ 1         6         11  14  16        21        26
                                    G C U G G G C G C A G G C C U G A C G G U A C A G C
/1duq_rnakbnm_decoy0008_amb_clx//A/ 1         6         11  /B/14  16        21        26
                                    G C U G G G C G C A G G    C C U G A C G G U A C A G C
```



13.4 Example #4 Calculate RMSDs of unstandardized structures (RNA Puzzle #1)

You try to calculate RMSDs for RNA Puzzles #1:

```
$ rna_calc_rmsd.py -t 1_solution_0_rpr.pdb *.pdb
method: all-atom-built-in
# of models: 15
1_bujnicki_1_rpr.pdb 5.71 978
1_bujnicki_2_rpr.pdb 6.16 978
1_bujnicki_3_rpr.pdb 5.3 978
1_bujnicki_4_rpr.pdb 4.95 978
1_bujnicki_5_rpr.pdb 5.1 978
```

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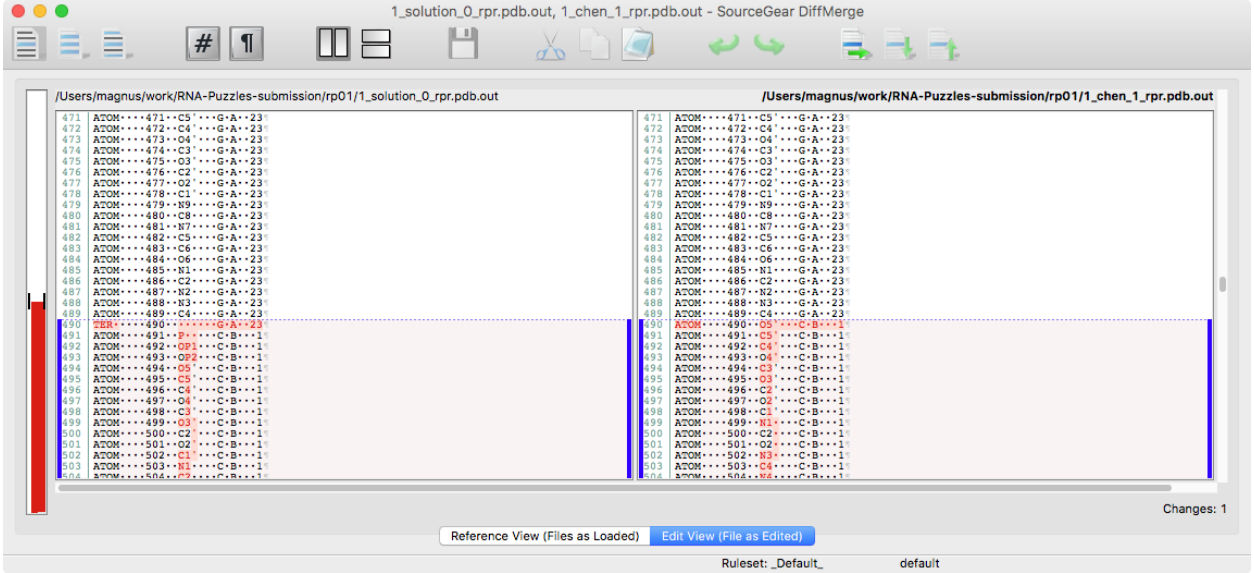
```
Error: # of atoms is not equal target (1_solution_0_rpr.pdb):978 vs model (1_chen_1_rpr.
↪pdb):975
```

you can see that there is a different number of atoms in *1_solution_0_rpr.pdb* and *1_chen_1_rpr.pdb*.

To see more you can run *diffpdb*.



you see that something is wrong. To fix it, run:

```
$ rna_pdb_tools.py --rpr --inplace *.pdb
93% (15 of 16) |#########################################################################################
↪################################################        | Elapsed Time: 0:00:03 ETA:␣
↪0:00:00
```

you can tail the files:

```
$ tail *.pdb
==> 1_bujnicki_1_rpr.pdb <==
ATOM    971  N7    G B  23     -16.558  -3.375  78.345  1.00  0.00           N
ATOM    972  C5    G B  23     -17.169  -2.575  77.384  1.00  0.00           C
ATOM    973  C6    G B  23     -17.589  -2.874  76.053  1.00  0.00           C
ATOM    974  O6    G B  23     -17.497  -3.930  75.430  1.00  0.00           O
ATOM    975  N1    G B  23     -18.234  -1.800  75.459  1.00  0.00           N
ATOM    976  C2    G B  23     -18.441  -0.576  76.049  1.00  0.00           C
ATOM    977  N2    G B  23     -19.127   0.345  75.382  1.00  0.00           N
ATOM    978  N3    G B  23     -18.053  -0.282  77.292  1.00  0.00           N
ATOM    979  C4    G B  23     -17.419  -1.324  77.898  1.00  0.00           C

...

==> 1_chen_1_rpr.pdb <==
ATOM    971  N7    G B  23     -14.462  -1.101  79.998  1.00  0.00           N
ATOM    972  C5    G B  23     -14.952  -0.485  78.839  1.00  0.00           C
ATOM    973  C6    G B  23     -15.577  -1.020  77.655  1.00  0.00           C
ATOM    974  O6    G B  23     -15.822  -2.189  77.351  1.00  0.00           O
```

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```
ATOM    975  N1    G B  23     -15.972  -0.051  76.763  1.00  0.00           N
ATOM    976  C2    G B  23     -15.787   1.274  76.944  1.00  0.00           C
ATOM    977  N2    G B  23     -16.269   2.059  76.021  1.00  0.00           N
ATOM    978  N3    G B  23     -15.224   1.822  78.022  1.00  0.00           N
ATOM    979  C4    G B  23     -14.818   0.884  78.935  1.00  0.00           C
TER     980        G B  23

==> 1_solution_0_rpr.pdb <==
ATOM    971  N7    G B  23      22.256  -1.292  27.403  1.00 34.10           N
ATOM    972  C5    G B  23      22.625  -0.176  28.135  1.00 31.12           C
ATOM    973  C6    G B  23      23.470  -0.096  29.260  1.00 28.80           C
ATOM    974  O6    G B  23      24.062  -1.036  29.804  1.00 28.26           O
ATOM    975  N1    G B  23      23.616   1.224  29.705  1.00 27.28           N
ATOM    976  C2    G B  23      22.971   2.318  29.112  1.00 28.31           C
ATOM    977  N2    G B  23      23.179   3.538  29.655  1.00 27.03           N
ATOM    978  N3    G B  23      22.170   2.245  28.047  1.00 28.85           N
ATOM    979  C4    G B  23      22.041   0.961  27.632  1.00 28.58           C
TER     980        G B  23%
```

so now you can see that the files look the same. Let's try to calculate RMSDs again:

```
$ rna_calc_rmsd.py -t 1_solution_0_rpr.pdb *.pdb
method: all-atom-built-in
# of models: 16
1_bujnicki_1_rpr.pdb 5.71 978
1_bujnicki_2_rpr.pdb 6.16 978
1_bujnicki_3_rpr.pdb 5.3 978
1_bujnicki_4_rpr.pdb 4.95 978
1_bujnicki_5_rpr.pdb 5.1 978
1_chen_1_rpr.pdb 4.35 978
1_chen_1_rpr_v2.pdb 4.35 978
1_das_1_rpr.pdb 3.97 978
1_das_2_rpr.pdb 4.48 978
1_das_3_rpr.pdb 3.43 978
1_das_4_rpr.pdb 3.92 978
1_das_5_rpr.pdb 4.57 978
1_dokholyan_1_rpr.pdb 7.25 978
1_major_1_rpr.pdb 4.34 978
1_santalucia_1_rpr.pdb 5.76 978
1_solution_0_rpr.pdb 0.0 978
# of atoms used: 978
csv was created!  rmsds.csv
```

worked! :-)

This is a real-life case, https://github.com/mmagnus/RNA-Puzzles-Normalized-submissions/tree/master/rp01.

CHAPTER

FOURTEEN

INSTALL & CONFIGURE

14.1 Pip as a developer

You can get rna-tools and install them from the current directory with this pip:

```
pip install -e git+http://github.com/mmagnus/rna-tools.git#egg=rna-tools
```

This way is better (than `pip install rna-tools`) if you're going to do some coding in the tools.

You can even first get rna-tools with git:

```
git clone http://github.com/mmagnus/rna-tools.git
```

and then do:

```
$ pip install -e .
Obtaining file:///Users/magnus/work/src/rna-tools
```

to "install" with pip rna-tools based on a set of links to the current directory.

14.2 Test if installed

Test if the package is installed:

```
$ python -c 'import rna_tools'
# ipython -c 'import rna_tools.tools.rna_calc_rmsd.rna_calc_rmsd' (to test specific␣
↪tools)
```

if nothing appears that's good. If you see this:

```
$ python -c 'import rna_tools'
Traceback (most recent call last):
  File "<string>", line 1, in <module>
ImportError: No module named rna_tools
```

then go to your config file for the shell (~/.zshrc or ~/.bashrc) add add:

```
PYTHONPATH=<path to rna-tools>/:$PYTHONPATH
export PYTHONPATH
```

so in my case this is:

```
PYTHONPATH=<path to rna-tools>/home/magnus/src/rna-tools/:$PYTHONPATH
export PYTHONPATH
```

14.3 Configuration

To set up your own configuration, create ~/.rna_tools.py in your HOME directory and redefine variables, e.g.:

```
(py37) [mx] rna-tools$ git:(master)  cat ~/.rna_tools.py
VARNA_PATH = '/Users/magnus/work/opt/varna'
VARNA_JAR_NAME = 'VARNA.jar'
SIMRNA_DATA_PATH = '/Users/magnus/work/opt/simRNA/SimRNA_64bitIntel_MacOSX_staticLibs/
↪data'
QRNAS_PATH = "/Users/magnus/work/opt/qrnas/"
RCHIE_PATH = "/Users/magnus/work/opt/r-chie/"
RFAM_DB_PATH = "/Users/magnus/work/db/rfam/Rfam.cm"
CONTEXTFOLD_PATH = "/Users/magnus/work/opt/ContextFold_1_00/"
DIFF_TOOL = "open -a diffmerge"
CPUS_CLUSTER = 630
RNASTRUCTURE_PATH = "/Users/magnus/work/opt/RNAstructure/6.1/"
ENTRNA_PATH = "/Users/magnus/work/opt/ENTRNA"
```

14.4 All requirements

To get ALL requirements, use `pip`:

```
pip install -r docs/requirements.txt
```

Be default rna-tools will not install all requirements, because some of them are heavy or might cause various problems, so you will be asked to install them when needed. For example, installing *matplotlib* is not essential for many other tools, *python-Levenshtein* is only used in one function.

14.5 Test all

This is still under active development.

To test (almost) all rna-tools functionality, you can run `rna_tools_test_all.py` to see if you got any errors, this should look like:

```
(py37) [mm] rna-tools$ git:(master) rna_tools_test_all.py
BlastPDB requires urllib3
- Python: 3.7.4 (default, Aug 13 2019, 15:17:50) [Clang 4.0.1 (tags/RELEASE_401/final)]
- rna-tools: b'py2-78-g3b3dd5f'
- RNA_TOOLS_PATH set to  /home/magnus/work-src/rna-tools/
- See full list of tools <https://github.com/mmagnus/rna-tools/blob/master/rna-tools-
↪index.csv
Seems OK
```

or for Python 2:

```
(base) [mm] rna-tools$ git:(master) rna_tools_test_all.py
- Python: 2.7.16 |Anaconda, Inc.| (default, Mar 14 2019, 16:24:02) [GCC 4.2.1 Compatible␣
↪Clang 4.0.1 (tags/RELEASE_401/final)]
- rna-tools: py2-78-g3b3dd5f
- RNA_TOOLS_PATH set to  /home/magnus/work-src/rna-tools/
- See full list of tools <https://github.com/mmagnus/rna-tools/blob/master/rna-tools-
↪index.csv
Seems OK
```

For crude testing you can also use `./test.sh` script and then see for errors in output and also check output/ folder to see if there are differences between your output and output committed to GitHub by me.

14.6 PyMOL4RNA: adv config

For some extra functions you migth also follow this. Open your *~/.pymolrc* and set up following variables as you need:

```
# rna-tools
EXECUTABLE="/bin/zsh" # set up your shell, usually /bin/bash or /bin/zsh
SOURCE="source ~/.zshrc" # set up the path to the file where you keep your shell␣
↪variables

CLARNA_RUN="/Users/magnus/work-src/clarna_play/clarna_run.py"  # if you want to run␣
↪clarna_run.py set up the path

run ~/work-src/rna-tools/rna_tools/tools/pymol_drawing/pymol_drawing.py
run ~/work-src/rna-tools/rna_tools/tools/rna_filter/pymol_dists.py
```

The plugins have been tested with MacPyMOL version 1.7.4.5 Edu.

CHAPTER

FIFTEEN

GIT QUICKREF

For Git in a scientific environment, please read:

> Perez-Riverol, Y. et al., 2016. Ten Simple Rules for Taking Advantage of Git and GitHub S. Markel, ed. PLoS computational biology, 12(7), p.e1004947.
>
> Blischak, J.D., Davenport, E.R. & Wilson, G., 2016. A Quick Introduction to Version Control with Git and GitHub F. Ouellette, ed. PLoS computational biology, 12(1), pp.e1004668–18.

Git is a version control system that is used for software development that helps you to keep track of versions of your program. To start using git you have to know only these two commands below. If you want to contribute to the package you need a few more, but it's not important right now :-)

To get the package for the first time on your computer go to the selected package and on the top left corner select clone or download. Copy the link and run it on console with git clone:

```
$ git clone git@github.com:mmagnus/rna-pdb-tools.git
```

and if you want to update the package later run:

```
$ git pull # be in the folder like ~/src/rna-pdb-tools/ <here>
```

if you see something like this:

```
$ git pull
Already up-to-date.
```

it means that your version of the package is up to date, congrats! :-)

If you see something like this:

```
 $ git pull
remote: Counting objects: 3, done.
remote: Compressing objects: 100% (1/1), done.
remote: Total 3 (delta 2), reused 3 (delta 2), pack-reused 0
Unpacking objects: 100% (3/3), done.
From github.com:mmagnus/rna-pdb-tools
```

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```
  69c4ee3..7f90739  master     -> origin/master
Updating 69c4ee3..7f90739
Fast-forward
install_links_bin.sh | 1 +
1 file changed, 1 insertion(+)
```

it means that there is a small change in `install_links_bin.sh` and you are up to date, congrats as well! You might need to run `./install_links_bin.sh` to "install" new tools that were added to the packages (if this is the case). If you get any error then talk to me `magnus@genesilico.pl`.

15.1 Git sheet cheat

```
$ git init # start git repo in a folder
$ git add <file> # add file to stage area
$ git commit -m <text> # send file to
$ git push # sent this remote
$ git gui # install `apt-get install git-gui`
$ git log #
$ git status # get status of your repo

$ git clone git@gitlab.genesilico.pl:magnus/git_crash_course.git

$ git remote add origin git@gitlab.genesilico.pl:magnus/git_crash_course.git

$ git push -u origin master
Counting objects: 45, done.
Delta compression using up to 8 threads.
Compressing objects: 100% (41/41), done.
Writing objects: 100% (45/45), 4.97 KiB | 0 bytes/s, done.
Total 45 (delta 12), reused 0 (delta 0)
To git@gitlab.genesilico.pl:magnus/git_crash_course.git
* [new branch]      master -> master
  Branch master set up to track remote branch master from origin.
```

15.2 Learn Git

Model used by Git vs Svn:

```
file <-> stage area <-> local repo <-> git repo/gitlab
file <-------------------------------> SVM repo
```

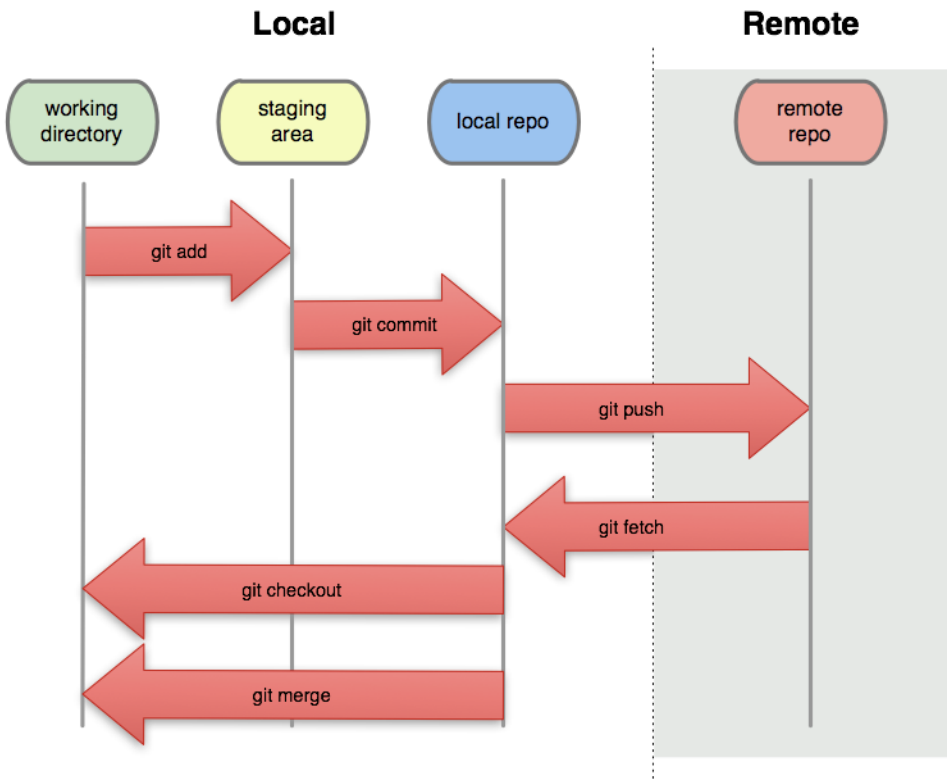


Figure. from: https://greenido.files.wordpress.com/2013/07/git-local-remote.png?w=696&h=570

For more see, git - the simple guide (just a simple guide for getting started with git. no deep shit ;))

http://rogerdudler.github.io/git-guide/

A git cheat sheet http://rogerdudler.github.io/git-guide/files/git_cheat_sheet.pdf .

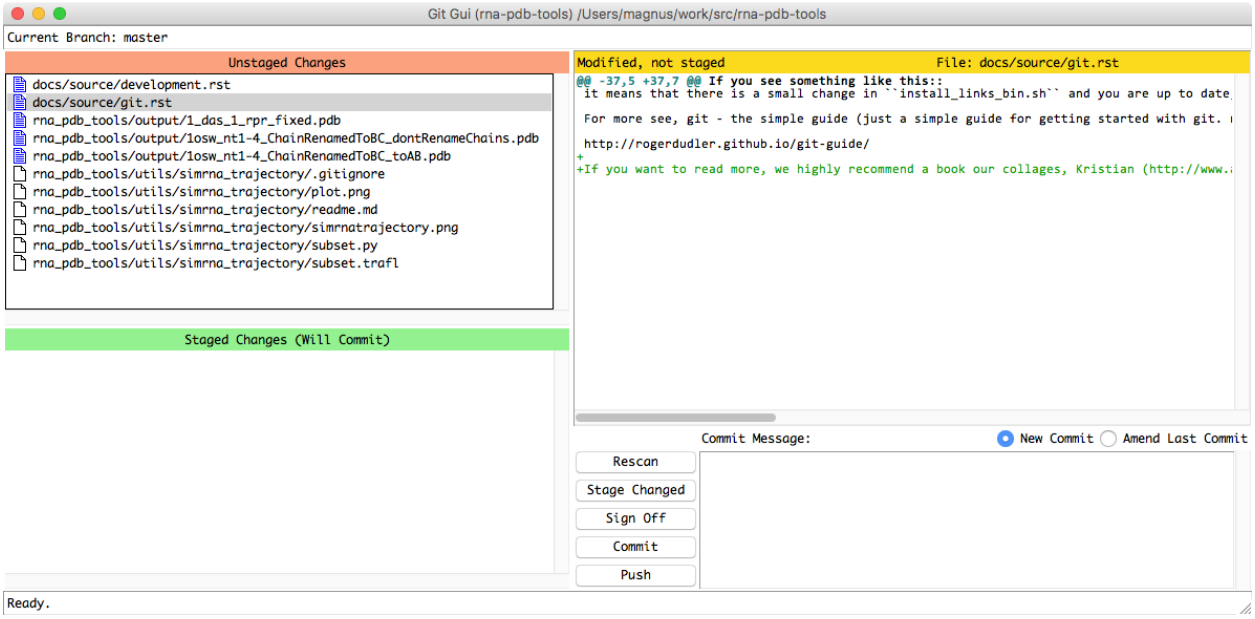
If you want to read more, we highly recommend a book our collages, Kristian (http://www.apress.com/us/book/9781484222409).

To understand the principles of Git, a bit more advance, by Linus Torvals (an author of Git) https://www.youtube.com/watch?v=4XpnKHJAok8)

How to learn Git in 20min https://www.youtube.com/watch?v=Y9XZQO1n_7c

15.3 Git GUI

You don't have to use terminal to work with git. Git comes with `git gui`.



You can also use `qgit` (http://sourceforge.net/projects/qgit/) and much more, a list of tools: https://git-scm.com/download/gui/linux .

CHAPTER

SIXTEEN

CONFIGURATION

Keep configuration sytanx like:

```
from rna_tools.rna_tools_config import CPUS_CLUSTER
# since we use export PYTHONPATH=$PYTHONPATH:/home/magnus/src/rna-tools/
```

vs:

```
try:
    RNA_ROSETTA_RUN_ROOT_DIR_MODELING = os.environ['RNA_ROSETTA_RUN_ROOT_DIR_MODELING']
except:
    print ('Set up RNA_ROSETTA_RUN_ROOT_DIR_MODELING in .bashrc')
```

CHAPTER

SEVENTEEN

DOCUMENTATION

We are using (at least we are moving towards)the Google style docstrings via Napoleon. Napoleon is a Sphinx Extensions that enables Sphinx to parse both NumPy and Google style docstrings - the style recommended by Khan Academy.
http://www.sphinx-doc.org/en/stable/ext/napoleon.html#type-annotations

17.1 Generate docs

At the moment the generation of the docs is quite tricky, because of old dependencies on Python2 and old version of Sphinx. To generate docs locally please switch to Python2 and then run `cd docs/; make clean; make html`.

It should be updated at some point.

CHAPTER

EIGHTEEN

ADD A NEW TOOL TO THE PACKAGE

1. Create a new folder in `rna-tools/rna_tools/tools` with your tool. The folder will be seen online after your push at https://github.com/mmagnus/rna-tools/tree/master/rna_tools/tools. We will walk you through this simple example https://github.com/mmagnus/rna-tools/tree/master/rna_tools/tools/renum_pdb_to_aln .
2. Make sure that there is a simple test as `test.sh`:

```
#!/bin/bash
python renum_pdb_to_aln.py --residue_index_start 1 obj1 test_data/ALN_OBJ1_OBJ2.fa␣
↪test_data/obj01.pdb
```

and there is a `test_data` folder with some test inputs and outputs. See the example.

3. Add your tool to `install_links_bin.sh` at the top folder of `rna-tools`:

```
ln -s $curr_dir/rna_tools /tools/<tool folder>/<util script name with .py> $curr_
↪dir/bin/<util script name with .py>

e.g.

ln -s $curr_dir/rnatools/utils/renum_pdb_to_aln/renum_pdb_to_aln.py $curr_dir/bin/
↪rna_renum_pdb_to_aln.py
```

This will "install" you script in bin directory of the project so it can be used system-wide.

Run this script to see if there is any error, `./install_links_bin.sh`.

4. Add your tool to the documentation. The tool has to be "importable", so don't forget to create `__init__.py` inside your tool directory. Next, go to `rna-tools/docs/source` and edit `tools.rst`. Add, wherever you think your tool will fit, lines like:

```
Renumber a pdb file according to alignment
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
.. autoprogram:: rna_tools.tools.<tool folder>.<tool script name>.get_parser()
   :prog: <utl script name>

.. automodule:: rna_tools.tools.<tool folder>.<tool script name>
   : members:

e.g.:

 Renumber a pdb file according to alignment
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
 .. autoprogram:: rna_tools.tools.renum_pdb_to_aln.renum_pdb_to_aln.get_parser()
```

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```
   :prog: renum_pdb_to_aln

.. automodule:: rna_tools.tools.renum_pdb_to_aln.renum_pdb_to_aln
  :members:
```

and run `make html` in the folder to check if the documentation is compiled without any errors.

If you are using any external library such us `scipy`, please make sure that they are listed in `rna-tools/docs/requirements.txt`. If the library is not there, please add it. This file is read by the Read The Docs to compile the documentation online and also by Travis for continuous testing.

You can open the documentation compiled locally under a link link file://<path to rna-tools>/rna-tools/docs/build/html/index.html, e.g. file:///Users/magnus/work/src/rna-tools/docs/build/html/index.html.

5. The very last step is to add your tool `test.sh` to the main testing script. Edit `rna-tools/test.sh` and add

```
cd ./tools/<tool folder>/
./test.sh
cd ../..

e.g.

cd ./tools/renum_pdb_to_aln/
./test.sh
cd ../..
```

6. Run this main test (`./test.sh`) and see if the tool works as expected.

7. Now we are ready to push the changes. In the terminal, type:

```
$ git pull
$ git add <files> # or use git gui
$ git commit -m <desc the tool>
$ git push
```

to commit all your changes and push it to the Github repository!

Warning: This testing is very, very rough and we are moving to have more test in py.test at some point.

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