

RNAlib-2.3.1

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Chapter 1

ViennaRNA Package core - RNAlib

A Library for folding and comparing RNA secondary structures

Date

1994-2016

Authors

Ivo Hofacker, Peter Stadler, Ronny Lorenz and many more

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1.1 Introduction

The core of the Vienna RNA Package ([10], [8]) is formed by a collection of routines for the prediction and comparison of RNA secondary structures. These routines can be accessed through stand-alone programs, such as RNAfold, RNAdistance etc., which should be sufficient for most users. For those who wish to develop their own programs we provide a library which can be linked to your own code.

This document describes the library and will be primarily useful to programmers. However, it also contains details about the implementation that may be of interest to advanced users. The stand-alone programs are described in separate man pages. The latest version of the package including source code and html versions of the documentation can be found at

<http://www.tbi.univie.ac.at/RNA/>

Chapter 2

Installation and Configuration of RNAlib Features

2.1 Installing the ViennaRNA Package

For best portability the ViennaRNA package uses the GNU autoconf and automake tools. The instructions below are for installing the ViennaRNA package from source. However, pre-compiled binaries for various Linux distributions, as well as for Windows users are available from Download section of the [main ViennaRNA homepage](#).

2.1.1 Quick-start

Usually you'll just unpack, configure and make. To do this type:

```
tar -zxvf ViennaRNA-2.2.8.tar.gz
cd ViennaRNA-2.2.8
./configure
make
sudo make install
```

2.1.2 Installation without root privileges

If you do not have root privileges on your computer, you might want to install the ViennaRNA Package to a location where you actually have write access to. To do so, you can set the installation prefix of the `./configure` script like so:

```
./configure --prefix=/home/username/ViennaRNA
make install
```

This will install the entire ViennaRNA Package into a new directory `ViennaRNA` directly into the users username home directory.

2.1.3 Notes for MacOS X users

Although users will find `/usr/bin/gcc` and `/usr/bin/g++` executables in their directory tree, these programs are not at all what they pretend to be. Instead of including the GNU programs, Apple decided to install clang/llvm in disguise. Unfortunately, the default version of clang/llvm does not support OpenMP (yet), but only complains at a late stage of the build process when this support is required. Therefore, it seems necessary to deactivate OpenMP support by passing the option `--disable-openmp` to the `./configure` script.

Additionally, since MacOS X 10.5 the perl and python installation distributed with MacOS X always include so called universal-binaries (a.k.a. fat-binaries), i.e. binaries for multiple architecture types. In order to compile and link the programs, library, and scripting language interfaces of the ViennaRNA Package for multiple architectures, we've added a new configure switch that sets up the required changes automatically:

```
./configure --enable-universal-binary
```

Note

Note, that with link time optimization turned on, MacOS X's default compiler (llvm/clang) generates an intermediary binary format that can not easily be combined into a multi-architecture library. Therefore, the `--enable-universal-binary` switch turns off link time optimization!

2.2 Configuring RNALib features

The ViennaRNA Package includes additional executable programs such as RNAforester, Kinfold, and Kinwalker. Furthermore, we include several features in our C-library that may be activated by default, or have to be explicitly turned on at configure-time. Below we list a selection of the available configure options that affect the features included in all executable programs, the RNALib C-library, and the corresponding scripting language interface(s).

2.2.1 Scripting Interfaces

The ViennaRNA Package comes with scripting language interfaces for Perl 5, Python 2, and Python 3 (provided by swig), that allow one to use the implemented algorithms directly without the need of calling an executable program. The interfaces are build by default whenever the autoconf tool-chain detects the required build tools on your system. You may, however, explicitly turn off particular scripting language interface support at configure-time, for instance for Perl 5 and Python 2, before the actual installation.

Example:

```
./configure --without-perl --without-python
```

Disabling the scripting language support all-together can be accomplished using the following switch:

```
./configure --without-swig
```

2.2.2 Cluster Analysis

The programs AnalyseSeqs and AnalyseDists offer some cluster analysis tools (split decomposition, statistical geometry, neighbor joining, Ward's method) for sequences and distance data. To also build these programs add

```
--with-cluster
```

to your configure options.

2.2.3 Kinfold

The Kinfold program can be used to simulate the folding dynamics of an RNA molecule, and is compiled by default. Use the

```
--without-kinfold
```

option to skip compilation and installation of Kinfold.

2.2.4 RNAforester

The RNAforester program is used for comparing secondary structures using tree alignment. Similar to Kinfold, use the

```
--without-forester
```

option to skip compilation and installation of RNAforester.

2.2.5 Kinwalker

The Kinwalker algorithm performs co-transcriptional folding of RNAs, starting at a user specified structure (default↵ : open chain) and ending at the minimum free energy structure. Compilation and installation of this program is deactivated by default. Use the

```
--with-kinwalker
```

option to enable building and installation of Kinwalker.

2.2.6 Link Time Optimization (LTO)

To increase the performance of our implementations, the ViennaRNA Package tries to make use of the Link Time Optimization (LTO) feature of modern C-compilers. If you are experiencing any troubles at make-time or run-time, or the configure script for some reason detects that your compiler supports this feature although it doesn't, you can deactivate it using the flag

```
./configure --disable-lto
```

2.2.7 OpenMP support

To enable concurrent computation of our implementations and in some cases parallelization of the algorithms we make use of the OpenMP API. This interface is well understood by most modern compilers. However, in some cases it might be necessary to deactivate OpenMP support and therefore transform *RNAlib* into a C-library that is not entirely *thread-safe*. To do so, add the following configure option

```
./configure --disable-openmp
```

2.2.8 Stochastic backtracking using Boustrophedon scheme

Stochastic backtracking for single RNA sequences, e.g. available through the RNAsubopt program, received a major speedup by implementing a Boustrophedon scheme (see this article for details). If for some reason you want to deactivate this feature, you can do that by adding the following switch to the configure script:

```
./configure --disable-boustrophedon
```

2.2.9 Generic Hard Constraints

The new constraints framework also implements first steps for generic hard constraints. However, this feature is deactivated by default due to performance reasons. Most users do not need this advanced feature since it is only accessible through the RNALib C-library. If you want to develop third-party programs that link against RNALib and make use of this feature, you need to enable it using by adding the following configure switch:

```
./configure --enable-gen-hard-constraints
```

2.2.10 SVM Z-score filter in RNALfold

By default, RNALfold that comes with the ViennaRNA Package allows for z-score filtering of its predicted results using a support vector machine (SVM). However, the library we use to implement this feature (libsvm) is statically linked to our own RNALib. If this introduces any problems for your own third-party programs that link against RNALib, you can safely switch off the z-scoring implementation using

```
./configure --without-svm
```

2.2.11 GNU Scientific Library

The new program RNApvmin computes a pseudo-energy perturbation vector that aims to minimize the discrepancy of predicted, and observed pairing probabilities. For that purpose it implements several methods to solve the optimization problem. Many of them are provided by the GNU Scientific Library, which is why the RNApvmin program, and the RNALib C-library are required to be linked against libgsl. If this introduces any problems in your own third-party programs that link against RNALib, you can turn off a larger portion of available minimizers in RN↔Apvmin and linking against libgsl all-together, using the switch

```
./configure --without-gsl
```

2.2.12 Disable C11/C++11 feature support

By default, we use C11/C++11 features in our implementations. This mainly accounts for unnamed unions/structs within *RNALib*. The configure script automatically detects whether or not your compiler understands these features. In case you are using an older compiler, these features will be deactivated by setting a specific pre-processor directive. If for some reason you want to deactivate C11/C++11 features despite the capabilities of your compiler, use the following configure option:

```
./configure --disable-c11
```


2.2.13 Enable warnings for use of deprecated symbols

Since version 2.2 we are in the process of transforming the API of our *RNAlib*. Hence, several symbols are marked as *deprecated* whenever they have been replaced by the new API. By default, deprecation warnings at compile time are deactivated. If you want to get your terminal spammed by tons of deprecation warnings, enable them using:

```
./configure --enable-warn-deprecated
```

2.2.14 Single precision partition function

Calculation of partition functions (via `RNAfold -p`) uses double precision floats by default, to avoid overflow errors on longer sequences. If your machine has little memory and you don't plan to fold sequences over 1000 bases in length you can compile the package to do the computations in single precision by running

```
./configure --enable-floatpf
```

Note

Using this option is discouraged and not necessary on most modern computers.

2.2.15 Help

For a complete list of all `./configure` options and important environment variables, type

```
./configure --help
```

For more general information on the build process see the `INSTALL.configure` file.

2.3 Linking against RNAlib

In order to use our implemented algorithms you simply need to link your program to our *RNAlib* C-library that usually comes along with the ViennaRNA Package installation. If you've installed the ViennaRNA Package as a pre-build binary package, you probably need the corresponding development package, e.g. *viennarna-devel*, or *viennarna-dev*. The only thing that is left is to include the ViennaRNA header files into your source code, e.g.:

```
#include <ViennaRNA/mfe.h>
```

and start using our fast and efficient algorithm implementations.

See also

In the [Examples](#) and [Some Examples using RNAlib API v3.0](#) sections, we list a small set of example code that usually is a good starting point for your application.

2.3.1 Compiler and Linker flags

Of course, simply adding the ViennaRNA header files into your source code is usually not enough. You probably need to tell your compiler where to find the header files, and sometimes add additional pre-processor directives. Whenever your installation of *RNAlib* was build with default settings and the header files were installed into their default location, a simple

```
-I/usr/include
```

pre-processor/compile flag should suffice. It can even be omitted in this case, since your compiler should search this directory by default anyway. You only need to change the path from */usr/include* to the correct location whenever the header files have been installed into a non-standard directory.

On the other hand, if you've compiled *RNAlib* with some non-default settings then you probably need to define some additional pre-processor macros:

- *WITH_GEN_HC* ... Enable the generic hard constraints API.

Warning

This directive should be added to your pre-processor/compile flags only if *RNAlib* was build with the *—enable-gen-hard-constraints* configure option.

See also

[Generic Hard Constraints](#) and [Hard constraints](#)

- *VRNA_DISABLE_C11_FEATURES* ... Disable C11/C++11 features.

Warning

Add this directive to your pre-processor/compile flags only if *RNAlib* was build with the *—disable-c11* configure option.

See also

[Disable C11/C++11 feature support](#) and [vrna_C11_features\(\)](#)

- *DEPRECATION_WARNINGS* ... Enable warnings for using deprecated symbols.

Note

Adding this directive enables compiler warnings whenever you use symbols in *RNAlib* that are marked *deprecated*.

See also

[Enable warnings for use of deprecated symbols](#) and [Deprecated List](#)

- *USE_FLOAT_PF* ... Use single precision floating point operations instead of double precision in partition function computations.

Warning

Define this macro only if *RNAlib* was build with the *—enable-floatpf* configure option!

See also

[Single precision partition function](#)

Simply add the corresponding definition(s) to your pre-processor/compile flags, for instance:

```
-DVRNA_DISABLE_C11_FEATURES
```

Finally, linking against *RNAlib* is achieved by adding the following linker flag

```
-L/usr/lib -lRNA -fopenmp
```

Again, the path to the library, */usr/lib*, may be omitted if this path is searched for libraries by default. The second flag tells the linker to include *libRNA.a*, and the remaining two flags activate [Link Time Optimization \(LTO\)](#) and [OpenMP support](#) support, respectively.

Note

Depending on your linker, the last two flags may differ.

Depending on your configure time decisions, you can drop one or both of the last flags.

In case you've compiled *RNAlib* with LTO support (See [Link Time Optimization \(LTO\)](#)) and you are using the same compiler for your third-party project that links against our library, you may add the

```
-flto
```

flag to enable Link Time Optimization.

2.3.2 The pkg-config tool

Instead of hard-coding the required compiler and linker flags, you can also let the *pkg-config* tool automatically determine the required flags. This tool is usually packaged for any Linux distribution and should be available for MacOS X and MinGW as well. We ship a file *RNAlib2.pc* which is installed along with the static *libRNA.a* C-library and populated with all required compiler and linker flags that correspond to your configure time decisions.

The compiler flags required for properly building your code that uses *RNAlib* can be easily obtained via

```
pkg-config --cflags RNAlib2
```

You get the corresponding linker flags using

```
pkg-config --libs RNAlib2
```

With this widely accepted standard it is also very easy to integrate *RNAlib* in your *autotools* project, just have a look at the *PKG_CHECK_MODULES* macro.

Chapter 3

Parsing and Comparing - Functions to Manipulate Structures

Representations of Secondary Structures

The standard representation of a secondary structure is the *bracket notation*, where matching brackets symbolize base pairs and unpaired bases are shown as dots. Alternatively, one may use two types of node labels, 'P' for paired and 'U' for unpaired; a dot is then replaced by '(U)', and each closed bracket is assigned an additional identifier 'P'. We call this the expanded notation. In [6] a condensed representation of the secondary structure is proposed, the so-called homeomorphically irreducible tree (HIT) representation. Here a stack is represented as a single pair of matching brackets labeled 'P' and weighted by the number of base pairs. Correspondingly, a contiguous strain of unpaired bases is shown as one pair of matching brackets labeled 'U' and weighted by its length. Generally any string consisting of matching brackets and identifiers is equivalent to a plane tree with as many different types of nodes as there are identifiers.

Bruce Shapiro proposed a coarse grained representation [17], which, does not retain the full information of the secondary structure. He represents the different structure elements by single matching brackets and labels them as 'H' (hairpin loop), 'I' (interior loop), 'B' (bulge), 'M' (multi-loop), and 'S' (stack). We extend his alphabet by an extra letter for external elements 'E'. Again these identifiers may be followed by a weight corresponding to the number of unpaired bases or base pairs in the structure element. All tree representations (except for the dot-bracket form) can be encapsulated into a virtual root (labeled 'R'), see the example below.

The following example illustrates the different linear tree representations used by the package. All lines show the same secondary structure.

```
a) .(((...(((...)))...((...))))).
   (U) ((( (U) (U) ((( (U) (U) (U) P) P) P) (U) (U) (( (U) (U) P) P) P) (U) P) P) (U)
b) (U) ((( (U2) ((U3) P3) (U2) ((U2) P2) P2) (U) P2) (U)
c) (( (H) (H) M) B)
   ((( (( (H) S) ((H) S) M) S) B) S)
   ((( ((( (H) S) ((H) S) M) S) B) S) E)
d) ((( ((( (( (H3) S3) ((H2) S2) M4) S2) B1) S2) E2) R)
```

Above: [Tree](#) representations of secondary structures. a) Full structure: the first line shows the more convenient condensed notation which is used by our programs; the second line shows the rather clumsy expanded notation for completeness, b) HIT structure, c) different versions of coarse grained structures: the second line is exactly Shapiro's representation, the first line is obtained by neglecting the stems. Since each loop is closed by a unique stem, these two lines are equivalent. The third line is an extension taking into account also the external digits. d) weighted coarse structure, this time including the virtual root.

For the output of aligned structures from string editing, different representations are needed, where we put the label on both sides. The above examples for tree representations would then look like:

- a) (UU) (P (P (P (P (UU) (UU) (P (P (P (UU) (UU) (UU) P) P) P) (UU) (UU) (P (P (UU) (U...))
- b) (UU) (P2 (P2 (U2U2) (P2 (U3U3) P3) (U2U2) (P2 (U2U2) P2) P2) (UU) P2) (UU)
- c) (B (M (HH) (HH) M) B)
 (S (B (S (M (S (HH) S) (S (HH) S) M) S) B) S)
 (E (S (B (S (M (S (HH) S) (S (HH) S) M) S) B) S) E)
- d) (R (E2 (S2 (B1 (S2 (M4 (S3 (H3) S3) ((H2) S2) M4) S2) B1) S2) E2) R)

Aligned structures additionally contain the gap character '_'.

Parsing and Coarse Graining of Structures

Several functions are provided for parsing structures and converting to different representations.

```
char *expand_Full(const char *structure)
```

Convert the full structure from bracket notation to the expanded notation including root.

```
char *b2HIT (const char *structure)
```

Converts the full structure from bracket notation to the HIT notation including root.

```
char *b2C (const char *structure)
```

Converts the full structure from bracket notation to the a coarse grained notation using the 'H' 'B' 'I' 'M' and 'R' identifiers.

```
char *b2Shapiro (const char *structure)
```

Converts the full structure from bracket notation to the *weighted* coarse grained notation using the 'H' 'B' 'I' 'M' 'S' 'E' and 'R' identifiers.

```
char *expand_Shapiro (const char *coarse);
```

Inserts missing 'S' identifiers in unweighted coarse grained structures as obtained from [b2C\(\)](#).

```
char *add_root (const char *structure)
```

Adds a root to an un-rooted tree in any except bracket notation.

```
char *unexpand_Full (const char *ffull)
```

Restores the bracket notation from an expanded full or HIT tree, that is any tree using only identifiers 'U' 'P' and 'R'.

```
char *unweight (const char *wcoarse)
```

Strip weights from any weighted tree.

```
void unexpand_aligned_F (char *align[2])
```

Converts two aligned structures in expanded notation.

```
void parse_structure (const char *structure)
```

Collects a statistic of structure elements of the full structure in bracket notation.

See also

[RNAstruct.h](#) for prototypes and more detailed description

Distance Measures

A simple measure of dissimilarity between secondary structures of equal length is the base pair distance, given by the number of pairs present in only one of the two structures being compared. I.e. the number of base pairs that have to be opened or closed to transform one structure into the other. It is therefore particularly useful for comparing structures on the same sequence. It is implemented by

```
int bp_distance(const char *str1,
               const char *str2)
```

Compute the "base pair" distance between two secondary structures s1 and s2.

For other cases a distance measure that allows for gaps is preferable. We can define distances between structures as edit distances between trees or their string representations. In the case of string distances this is the same as "sequence alignment". Given a set of edit operations and edit costs, the edit distance is given by the minimum sum of the costs along an edit path converting one object into the other. Edit distances like these always define a metric. The edit operations used by us are insertion, deletion and replacement of nodes. String editing does not pay attention to the matching of brackets, while in tree editing matching brackets represent a single node of the tree. [Tree](#) editing is therefore usually preferable, although somewhat slower. String edit distances are always smaller or equal to tree edit distances.

The different level of detail in the structure representations defined above naturally leads to different measures of distance. For full structures we use a cost of 1 for deletion or insertion of an unpaired base and 2 for a base pair. Replacing an unpaired base for a pair incurs a cost of 1.

Two cost matrices are provided for coarse grained structures:

```
/* Null,  H,  B,  I,  M,  S,  E  */
{ 0,  2,  2,  2,  2,  1,  1}, /* Null replaced */
{ 2,  0,  2,  2,  2,  INF, INF}, /* H   replaced */
{ 2,  2,  0,  1,  2,  INF, INF}, /* B   replaced */
{ 2,  2,  1,  0,  2,  INF, INF}, /* I   replaced */
{ 2,  2,  2,  2,  0,  INF, INF}, /* M   replaced */
{ 1,  INF, INF, INF, INF,  0, INF}, /* S   replaced */
{ 1,  INF, INF, INF, INF,  INF,  0}, /* E   replaced */

/* Null,  H,  B,  I,  M,  S,  E  */
{ 0, 100,  5,  5,  75,  5,  5}, /* Null replaced */
{ 100,  0,  8,  8,  8,  INF, INF}, /* H   replaced */
{  5,  8,  0,  3,  8,  INF, INF}, /* B   replaced */
{  5,  8,  3,  0,  8,  INF, INF}, /* I   replaced */
{ 75,  8,  8,  8,  0,  INF, INF}, /* M   replaced */
{  5,  INF, INF, INF, INF,  0, INF}, /* S   replaced */
{  5,  INF, INF, INF, INF,  INF,  0}, /* E   replaced */
```

The lower matrix uses the costs given in [18]. All distance functions use the following global variables:

```
int cost_matrix;
```

Specify the cost matrix to be used for distance calculations.

```
int edit_backtrack;
```

Produce an alignment of the two structures being compared by tracing the editing path giving the minimum distance.

```
char *aligned_line[4];
```

Contains the two aligned structures after a call to one of the distance functions with [edit_backtrack](#) set to 1.

See also

[utils.h](#), [dist_vars.h](#) and [stringdist.h](#) for more details

Functions for [Tree](#) Edit Distances

```
Tree    *make_tree (char *struc)
```

Constructs a [Tree](#) (essentially the postorder list) of the structure 'struc', for use in [tree_edit_distance\(\)](#).

```
float    tree_edit_distance (Tree *T1,  
                             Tree *T2)
```

Calculates the edit distance of the two trees.

```
void     free_tree(Tree *t)
```

Free the memory allocated for [Tree](#) t.

See also

[dist_vars.h](#) and [treedist.h](#) for prototypes and more detailed descriptions

Functions for String Alignment

```
swString *Make_swString (char *string)
```

Convert a structure into a format suitable for [string_edit_distance\(\)](#).

```
float     string_edit_distance (swString *T1,  
                               swString *T2)
```

Calculate the string edit distance of T1 and T2.

See also

[dist_vars.h](#) and [stringdist.h](#) for prototypes and more detailed descriptions

Functions for Comparison of Base Pair Probabilities

For comparison of base pair probability matrices, the matrices are first condensed into probability profiles which are then compared by alignment.

```
float *Make_bp_profile_bppm ( double *bppm,  
                             int length)
```

condense pair probability matrix into a vector containing probabilities for unpaired, upstream paired and downstream paired.

```
float profile_edit_distance ( const float *T1,  
                             const float *T2)
```

Align the 2 probability profiles T1, T2

.

See also

[ProfileDist.h](#) for prototypes and more details of the above functions

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Chapter 4

Utilities - Odds and Ends

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4.1 Producing secondary structure graphs

```
int PS_rna_plot ( char *string,
                  char *structure,
                  char *file)
```

Produce a secondary structure graph in PostScript and write it to 'filename'.

```
int PS_rna_plot_a (
    char *string,
    char *structure,
    char *file,
    char *pre,
    char *post)
```

Produce a secondary structure graph in PostScript including additional annotation macros and write it to 'filename'.

```
int gmlRNA (char *string,
            char *structure,
            char *ssfile,
            char option)
```

Produce a secondary structure graph in Graph Meta Language (gml) and write it to a file.

```
int ssv_rna_plot (char *string,
                 char *structure,
                 char *ssfile)
```

Produce a secondary structure graph in SStructView format.

```
int svg_rna_plot (char *string,
                 char *structure,
                 char *ssfile)
```

Produce a secondary structure plot in SVG format and write it to a file.

```
int xrna_plot ( char *string,
                char *structure,
                char *ssfile)
```

Produce a secondary structure plot for further editing in XRNA.

```
int rna_plot_type
```

Switch for changing the secondary structure layout algorithm.

Two low-level functions provide direct access to the graph lauyouting algorithms:

```
int simple_xy_coordinates ( short *pair_table,
                           float *X,
                           float *Y)
```

Calculate nucleotide coordinates for secondary structure plot the *Simple way*

```
int naview_xy_coordinates ( short *pair_table,
                           float *X,
                           float *Y)
```

See also

[PS_dot.h](#) and [naview.h](#) for more detailed descriptions.

4.2 Producing (colored) dot plots for base pair probabilities

```
int PS_color_dot_plot ( char *string,
                       cpair *pi,
                       char *filename)
```

```
int PS_color_dot_plot_turn (char *seq,
                           cpair *pi,
                           char *filename,
                           int winSize)
```

```
int PS_dot_plot_list (char *seq,
                     char *filename,
                     plist *pl,
                     plist *mf,
                     char *comment)
```

Produce a postscript dot-plot from two pair lists.

```
int PS_dot_plot_turn (char *seq,
                     struct plist *pl,
                     char *filename,
                     int winSize)
```

See also

[PS_dot.h](#) for more detailed descriptions.

4.3 Producing (colored) alignments

```
int PS_color_aln (
    const char *structure,
    const char *filename,
    const char *seqs[],
    const char *names[])
```

Produce PostScript sequence alignment color-annotated by consensus structure.

4.4 RNA sequence related utilities

Several functions provide useful applications to RNA sequences

```
char *random_string (int l,
                     const char symbols[])
```

Create a random string using characters from a specified symbol set.

```
int hamming ( const char *s1,
              const char *s2)
```

Calculate hamming distance between two sequences.

```
void str_DNA2RNA(char *sequence);
```

Convert a DNA input sequence to RNA alphabet.

```
void str_uppercase(char *sequence);
```

Convert an input sequence to uppercase.

4.5 RNA secondary structure related utilities

```
char *pack_structure (const char *struc)
```

Pack secondary structure, 5:1 compression using base 3 encoding.

```
char *unpack_structure (const char *packed)
```

Unpack secondary structure previously packed with [pack_structure\(\)](#)

```
short *make_pair_table (const char *structure)
```

Create a pair table of a secondary structure.

```
short *copy_pair_table (const short *pt)
```

Get an exact copy of a pair table.

4.6 Miscellaneous Utilities

```
void print_tty_input_seq (void)
```

Print a line to *stdout* that asks for an input sequence.

```
void print_tty_constraint_full (void)
```

Print structure constraint characters to *stdout* (full constraint support)

```
void print_tty_constraint (unsigned int option)
```

Print structure constraint characters to *stdout*. (constraint support is specified by option parameter)

```
int  *get_iidx (unsigned int length)
```

```
int  *get_idx (unsigned int length)
```

```
void constrain_ptypes (
    const char *constraint,
    unsigned int length,
    char *ptype,
    int *BP,
    int min_loop_size,
    unsigned int idx_type)
```

Insert constraining pair types according to constraint structure string.

```
char  *get_line(FILE *fp);
```

Read a line of arbitrary length from a stream.

```
unsigned int read_record(
    char **header,
    char **sequence,
    char ***rest,
    unsigned int options);
```

Get a data record from *stdin*.

```
char  *time_stamp (void)
```

Get a timestamp.

```
void warn_user (const char message[])
```

Print a warning message.

```
void nrerror (const char message[])
```

Die with an error message.

```
void    init_rand (void)
```

Make random number seeds.

```
unsigned short xsubi[3];
```

Current 48 bit random number.

```
double urn (void)
```

get a random number from [0..1]

```
int      int_urn (int from, int to)
```

Generates a pseudo random integer in a specified range.

```
void     *space (unsigned size)
```

Allocate space safely.

```
void     *xrealloc ( void *p,  
                    unsigned size)
```

Reallocate space safely.

See also

[utils.h](#) for a complete overview and detailed description of the utility functions

[Next Page: The new RNAlib API v3.0](#)

Chapter 5

RNAlib API v3.0

5.1 Introduction

With version 2.2 we introduce the new API that will take over the old one in the future version 3.0. By then, backwards compatibility will be broken, and third party applications using RNAlib need to be ported. This switch of API became necessary, since many new features found their way into the RNAlib where a balance between threadsafety and easy-to-use library functions is hard or even impossible to establish. Furthermore, many old functions of the library are present as slightly modified copies of themselves to provide a crude way to overload functions.

Therefore, we introduce the new v3.0 API very early in our development stage such that developers have enough time to migrate to the new functions and interfaces. We also started to provide encapsulation of the RNAlib functions, data structures, typedefs, and macros by prefixing them with *vrna_* and *VRNA_*, respectively. Header files should also be included using the *ViennaRNA/* namespace, e.g.

```
#include <ViennaRNA/fold.h>
```

instead of just using

```
#include <fold.h>
```

as required for RNAlib 1.x and 2.x.

This eases the work for programmers of third party applications that would otherwise need to put much effort into renaming functions and data types in their own implementations if their names appear in our library. Since we still provide backward compatibility up to the last version of RNAlib 2.x, this advantage may be fully exploited only starting from v3.0 which will be released in the future. However, our plan is to provide the possibility for an early switch-off mechanism of the backward compatibility in one of our next releases of ViennaRNA Package 2.x.

5.2 What are the major changes?

...

5.3 How to port your program to the new API

...

5.4 Some Examples using RNAlib API v3.0

Examples on how to use the new v3.0 API can be found in the [Using the 'new' v3.0 API](#) section.

Chapter 6

Scripting Language interface(s)

Notes on functions and structures wrapped to the scripting language interface(s)

6.1 Introduction

For an easy integration into scripting languages, we provide an automatically generated interface to the RNAlib C-library, generated with scripting.

6.2 Function renaming scheme

The main difference when using a scripting language interface compared to direct calls of RNAlib C functions is, that the prefix 'vrna_' is dropped. For instance, when calling the [vrna_fold\(\)](#) function, corresponding calls in perl or python are `RNA::fold()`, and `RNA.fold()`, respectively.

Functions that are dedicated to work on specific data structures only, e.g. the [vrna_fold_compound_t](#), are usually not exported at all. Instead, they are attached as object methods of a corresponding class (see [Object oriented Interface for data structures](#) for detailed information).

6.3 Object oriented Interface for data structures

For data structures, typedefs, and enumerations the 'vrna_' prefixes are dropped as well, together with their suffixes '_s', '_t', and '_e', respectively. Furthermore, data structures are usually transformed into classes and relevant functions of the C-library are attached as methods.

6.4 Examples

Examples on the basic usage of the scripting language interfaces can be found in the [Perl Examples](#) and [Python Examples](#) section.

6.5 Wrapper notes

Special notes on how functions, structures, enums, and macro definitions are actually wrapped, can be found here: [SWIG Wrapper Notes](#).

Chapter 7

SWIG Wrapper Notes

Below, you find an enumeration of special note on how functions, structures, enums, and macro definitions are wrapped.

Global **[vrna_commands_apply](#)** (**[vrna_fold_compound_t](#)** *vc, **[vrna_cmd_t](#)** *commands, unsigned int options)

This function is attached as method **commands_apply()** to objects of type *fold_compound*

Global **[vrna_enumerate_necklaces](#)** (const unsigned int *type_counts)

This function is available as global function **enumerate_necklaces()** which accepts lists input, and produces list of lists output.

Global **[vrna_eval_covar_structure](#)** (**[vrna_fold_compound_t](#)** *vc, const char *structure)

This function is attached as method **eval_covar_structure()** to objects of type *fold_compound*

Global **[vrna_eval_hp_loop](#)** (**[vrna_fold_compound_t](#)** *vc, int i, int j)

This function is attached as method **eval_hp_loop()** to objects of type *fold_compound*

Global **[vrna_eval_int_loop](#)** (**[vrna_fold_compound_t](#)** *vc, int i, int j, int k, int l)

This function is attached as method **eval_int_loop()** to objects of type *fold_compound*

Global **[vrna_eval_loop_pt](#)** (**[vrna_fold_compound_t](#)** *vc, int i, const short *pt)

This function is attached as method **eval_loop_pt()** to objects of type *fold_compound*

Global **[vrna_eval_move](#)** (**[vrna_fold_compound_t](#)** *vc, const char *structure, int m1, int m2)

This function is attached as method **eval_move()** to objects of type *fold_compound*

Global **[vrna_eval_move_pt](#)** (**[vrna_fold_compound_t](#)** *vc, short *pt, int m1, int m2)

This function is attached as method **eval_move_pt()** to objects of type *fold_compound*

Global **[vrna_eval_structure](#)** (**[vrna_fold_compound_t](#)** *vc, const char *structure)

This function is attached as method **eval_structure()** to objects of type *fold_compound*

Global **[vrna_eval_structure_pt](#)** (**[vrna_fold_compound_t](#)** *vc, const short *pt)

This function is attached as method **eval_structure_pt()** to objects of type *fold_compound*

Global **[vrna_eval_structure_pt_verbose](#)** (**[vrna_fold_compound_t](#)** *vc, const short *pt, FILE *file)

This function is attached as method **eval_structure_pt_verbose()** to objects of type *fold_compound*

Global **[vrna_eval_structure_verbose](#)** (**[vrna_fold_compound_t](#)** *vc, const char *structure, FILE *file)

This function is attached as method **eval_structure_verbose()** to objects of type *fold_compound*

Global `vrna_exp_params_rescale` (`vrna_fold_compound_t *vc`, `double *mfe`)

This function is attached to `vrna_fc_s` objects as overloaded `exp_params_rescale()` method.

When no parameter is passed to this method, the resulting action is the same as passing `NULL` as second parameter to `vrna_exp_params_rescale()`, i.e. default scaling of the partition function. Passing an energy in kcal/mol, e.g. as retrieved by a previous call to the `mfe()` method, instructs all subsequent calls to scale the partition function accordingly.

Global `vrna_exp_params_reset` (`vrna_fold_compound_t *vc`, `vrna_md_t *md_p`)

This function is attached to `vrna_fc_s` objects as overloaded `exp_params_reset()` method.

When no parameter is passed to this method, the resulting action is the same as passing `NULL` as second parameter to `vrna_exp_params_reset()`, i.e. global default model settings are used. Passing an object of type `vrna_md_s` resets the fold compound according to the specifications stored within the `vrna_md_s` object.

Class `vrna_fc_s`

This data structure is wrapped as an object `fold_compound` with several related functions attached as methods.

A new `fold_compound` can be obtained by calling one of its constructors:

- `fold_compound(seq)` – Initialize with a single sequence, or two concatenated sequences separated by an ampersand character '&' (for cofolding)
- `fold_compound(aln)` – Initialize with a sequence alignment `aln` stored as a list of sequences (with gap characters)

The resulting object has a list of attached methods which in most cases directly correspond to functions that mainly operate on the corresponding `C` data structure:

- `type()` – Get the type of the `fold_compound` (See `vrna_fc_type_e`)
- `length()` – Get the length of the sequence(s) or alignment stored within the `fold_compound`

Global `vrna_file_commands_apply` (`vrna_fold_compound_t *vc`, `const char *filename`, `unsigned int options`)

This function is attached as method `file_commands_apply()` to objects of type `fold_compound`

Global `vrna_hc_add_bp` (`vrna_fold_compound_t *vc`, `int i`, `int j`, `char option`)

This function is attached as method `hc_add_bp()` to objects of type `fold_compound`

Global `vrna_hc_add_bp_nonspecific` (`vrna_fold_compound_t *vc`, `int i`, `int d`, `char option`)

This function is attached as method `hc_add_bp_nonspecific()` to objects of type `fold_compound`

Global `vrna_hc_add_from_db` (`vrna_fold_compound_t *vc`, `const char *constraint`, `unsigned int options`)

This function is attached as method `hc_add_from_db()` to objects of type `fold_compound`

Global `vrna_hc_add_up` (`vrna_fold_compound_t *vc`, `int i`, `char option`)

This function is attached as method `hc_add_up()` to objects of type `fold_compound`

Global `vrna_hc_init` (`vrna_fold_compound_t *vc`)

This function is attached as method `hc_init()` to objects of type `fold_compound`

Class `vrna_md_s`

This data structure is wrapped as an object `md` with multiple related functions attached as methods.

A new set of default parameters can be obtained by calling the constructor of `md`:

- `md()` – Initialize with default settings

The resulting object has a list of attached methods which directly correspond to functions that mainly operate on the corresponding `C` data structure:

- `reset()` – `vrna_md_set_default()`

- `set_from_globals()` – `set_model_details()`
- `option_string()` – `vrna_md_option_string()`

Note, that default parameters can be modified by directly setting any of the following global variables. Internally, getting/setting default parameters using their global variable representative translates into calls of the following functions, therefore these wrappers for these functions do not exist in the scripting language interface(s):

global variable	C getter	C setter
temperature	<code>vrna_md_defaults_temperature_get()</code>	<code>vrna_md_defaults_temperature()</code>
dangles	<code>vrna_md_defaults_dangles_get()</code>	<code>vrna_md_defaults_dangles()</code>
betaScale	<code>vrna_md_defaults_betaScale_get()</code>	<code>vrna_md_defaults_betaScale()</code>
tetra_loop	this is an alias of <i>special_hp</i>	
special_hp	<code>vrna_md_defaults_special_hp_get()</code>	<code>vrna_md_defaults_special_hp()</code>
noLonelyPairs	this is an alias of <i>noLP</i>	
noLP	<code>vrna_md_defaults_noLP_get()</code>	<code>vrna_md_defaults_noLP()</code>
noGU	<code>vrna_md_defaults_noGU_get()</code>	<code>vrna_md_defaults_noGU()</code>
no_closingGU	this is an alias of <i>noGUclosure</i>	
noGUclosure	<code>vrna_md_defaults_noGUclosure_get()</code>	<code>vrna_md_defaults_noGUclosure()</code>
logML	<code>vrna_md_defaults_logML_get()</code>	<code>vrna_md_defaults_logML()</code>
circ	<code>vrna_md_defaults_circ_get()</code>	<code>vrna_md_defaults_circ()</code>
gquad	<code>vrna_md_defaults_gquad_get()</code>	<code>vrna_md_defaults_gquad()</code>
uniq_ML	<code>vrna_md_defaults_uniq_ML_get()</code>	<code>vrna_md_defaults_uniq_ML()</code>
energy_set	<code>vrna_md_defaults_energy_set_get()</code>	<code>vrna_md_defaults_energy_set()</code>
backtrack	<code>vrna_md_defaults_backtrack_get()</code>	<code>vrna_md_defaults_backtrack()</code>
backtrack_type	<code>vrna_md_defaults_backtrack_type_get()</code>	<code>vrna_md_defaults_backtrack_type()</code>
do_backtrack	this is an alias of <i>compute_bpp</i>	
compute_bpp	<code>vrna_md_defaults_compute_bpp_get()</code>	<code>vrna_md_defaults_compute_bpp()</code>
max_bp_span	<code>vrna_md_defaults_max_bp_span_get()</code>	<code>vrna_md_defaults_max_bp_span()</code>
min_loop_size	<code>vrna_md_defaults_min_loop_size_get()</code>	<code>vrna_md_defaults_min_loop_size()</code>
window_size	<code>vrna_md_defaults_window_size_get()</code>	<code>vrna_md_defaults_window_size()</code>
oldAliEn	<code>vrna_md_defaults_oldAliEn_get()</code>	<code>vrna_md_defaults_oldAliEn()</code>
ribo	<code>vrna_md_defaults_ribo_get()</code>	<code>vrna_md_defaults_ribo()</code>
cv_fact	<code>vrna_md_defaults_cv_fact_get()</code>	<code>vrna_md_defaults_cv_fact()</code>
nc_fact	<code>vrna_md_defaults_nc_fact_get()</code>	<code>vrna_md_defaults_nc_fact()</code>
sfact	<code>vrna_md_defaults_sfact_get()</code>	<code>vrna_md_defaults_sfact()</code>

Global `vrna_mean_bp_distance` (`vrna_fold_compound_t *vc`)

This function is attached as method `mean_bp_distance()` to objects of type *fold_compound*

Global `vrna_mfe` (`vrna_fold_compound_t *vc`, `char *structure`)

This function is attached as method `mfe()` to objects of type *fold_compound*

Global `vrna_mfe_dimer` (`vrna_fold_compound_t *vc`, `char *structure`)

This function is attached as method `mfe_dimer()` to objects of type *fold_compound*

Global `vrna_mfe_window` (`vrna_fold_compound_t *vc`, `FILE *file`)

This function is attached as method `mfe_window()` to objects of type *fold_compound*

Global `vrna_params_reset` (`vrna_fold_compound_t *vc`, `vrna_md_t *md_p`)

This function is attached to `vrna_fc_s` objects as overloaded `params_reset()` method.

When no parameter is passed to this method, the resulting action is the same as passing *NULL* as second parameter to `vrna_params_reset()`, i.e. global default model settings are used. Passing an object of type `vrna_md_s` resets the fold compound according to the specifications stored within the `vrna_md_s` object.

Global **vrna_params_subst** (vrna_fold_compound_t *vc, vrna_param_t *par)

This function is attached to **vrna_fc_s** objects as **params_subst()** method.

Global **vrna_pf** (vrna_fold_compound_t *vc, char *structure)

This function is attached as method **pf()** to objects of type *fold_compound*

Global **vrna_pf_dimer** (vrna_fold_compound_t *vc, char *structure)

This function is attached as method **pf_dimer()** to objects of type *fold_compound*

Global **vrna_sc_add_bp** (vrna_fold_compound_t *vc, int i, int j, FLT_OR_DBL energy, unsigned int options)

This function is attached as an overloaded method **sc_add_bp()** to objects of type *fold_compound*. The method either takes arguments for a single base pair (i,j) with the corresponding energy value:

```
fold_compound.sc_add_bp(i, j, energy, options)
```

or an entire 2-dimensional matrix with dimensions $n \times n$ that stores free energy contributions for any base pair (i,j) with $1 \leq i < j \leq n$:

```
fold_compound.sc_add_bp(matrix, options)
```

In both variants, the **options** argument is optional can may be omitted.

Global **vrna_sc_add_bt** (vrna_fold_compound_t *vc, vrna_callback_sc_backtrack *f)

This function is attached as method **sc_add_bt()** to objects of type *fold_compound*

Global **vrna_sc_add_data** (vrna_fold_compound_t *vc, void *data, vrna_callback_free_auxdata *free_data)

This function is attached as method **sc_add_data()** to objects of type *fold_compound*

Global **vrna_sc_add_exp_f** (vrna_fold_compound_t *vc, vrna_callback_sc_exp_energy *exp_f)

This function is attached as method **sc_add_exp_f()** to objects of type *fold_compound*

Global **vrna_sc_add_f** (vrna_fold_compound_t *vc, vrna_callback_sc_energy *f)

This function is attached as method **sc_add_f()** to objects of type *fold_compound*

Global **vrna_sc_add_hi_motif** (vrna_fold_compound_t *vc, const char *seq, const char *structure, FLT_OR_DBL energy, unsigned int options)

This function is attached as method **sc_add_hi_motif()** to objects of type *fold_compound*

Global **vrna_sc_add_SHAPE_deigan** (vrna_fold_compound_t *vc, const double *reactivities, double m, double b, unsigned int options)

This function is attached as method **sc_add_SHAPE_deigan()** to objects of type *fold_compound*

Global **vrna_sc_add_SHAPE_deigan_ali** (vrna_fold_compound_t *vc, const char **shape_files, const int *shape_file_association, double m, double b, unsigned int options)

This function is attached as method **sc_add_SHAPE_deigan_ali()** to objects of type *fold_compound*

Global **vrna_sc_add_SHAPE_zarringhalam** (vrna_fold_compound_t *vc, const double *reactivities, double b, double default_value, const char *shape_conversion, unsigned int options)

This function is attached as method **sc_add_SHAPE_zarringhalam()** to objects of type *fold_compound*

Global **vrna_sc_add_up** (vrna_fold_compound_t *vc, int i, FLT_OR_DBL energy, unsigned int options)

This function is attached as an overloaded method **sc_add_up()** to objects of type *fold_compound*. The method either takes arguments for a single nucleotide *i* with the corresponding energy value:

```
fold_compound.sc_add_up(i, energy, options)
```

or an entire vector that stores free energy contributions for each nucleotide *i* with $1 \leq i \leq n$:

```
fold_compound.sc_add_bp(vector, options)
```

In both variants, the **options** argument is optional can may be omitted.

Global **vrna_sc_init** (vrna_fold_compound_t *vc)

This function is attached as method **sc_init()** to objects of type *fold_compound*

Global **vrna_sc_remove** (vrna_fold_compound_t *vc)

This function is attached as method **sc_remove()** to objects of type *fold_compound*

Global **vrna_sc_set_bp** (vrna_fold_compound_t *vc, const FLT_OR_DBL **constraints, unsigned int options)

This function is attached as method **sc_set_bp()** to objects of type *fold_compound*

Global **vrna_sc_set_up** (vrna_fold_compound_t *vc, const FLT_OR_DBL *constraints, unsigned int options)

This function is attached as method **sc_set_up()** to objects of type *fold_compound*

Global **vrna_subopt** (vrna_fold_compound_t *vc, int delta, int sorted, FILE *fp)

This function is attached as method **subopt()** to objects of type *fold_compound*

Global **vrna_subopt_cb** (vrna_fold_compound_t *vc, int delta, vrna_subopt_callback *cb, void *data)

This function is attached as method **subopt_cb()** to objects of type *fold_compound*

Global **vrna_subopt_zuker** (vrna_fold_compound_t *vc)

This function is attached as method **subopt_zuker()** to objects of type *fold_compound*

Global **vrna_ud_add_motif** (vrna_fold_compound_t *vc, const char *motif, double motif_en, unsigned int loop_type)

This function is attached as method **ud_add_motif()** to objects of type *fold_compound*

Global **vrna_ud_remove** (vrna_fold_compound_t *vc)

This function is attached as method **ud_remove()** to objects of type *fold_compound*

Global **vrna_ud_set_data** (vrna_fold_compound_t *vc, void *data, vrna_callback_free_auxdata *free_cb)

This function is attached as method **ud_set_data()** to objects of type *fold_compound*

Global **vrna_ud_set_exp_prod_rule_cb** (vrna_fold_compound_t *vc, vrna_callback_ud_exp_production *pre_cb, vrna_callback_ud_exp_energy *exp_e_cb)

This function is attached as method **ud_set_exp_prod_rule_cb()** to objects of type *fold_compound*

Global **vrna_ud_set_prob_cb** (vrna_fold_compound_t *vc, vrna_callback_ud_probs_add *setter, vrna_callback_ud_probs_get *getter)

This function is attached as method **ud_set_prob_cb()** to objects of type *fold_compound*

Global **vrna_ud_set_prod_rule_cb** (vrna_fold_compound_t *vc, vrna_callback_ud_production *pre_cb, vrna_callback_ud_energy *e_cb)

This function is attached as method **ud_set_prod_rule_cb()** to objects of type *fold_compound*

Chapter 8

Input / Output File Formats

8.1 File formats for Multiple Sequence Alignments (MSA)

8.1.1 ClustalW format

The *ClustalW* format is a relatively simple text file containing a single multiple sequence alignment of DNA, RNA, or protein sequences. It was first used as an output format for the *clustalw* programs, but nowadays it may also be generated by various other sequence alignment tools. The specification is straight forward:

- The first line starts with the words

```
CLUSTAL W
```

or

```
CLUSTALW
```

- After the above header there is at least one empty line
- Finally, one or more blocks of sequence data are following, where each block is separated by at least one empty line

Each line in a blocks of sequence data consists of the sequence name followed by the sequence symbols, separated by at least one whitespace character. Usually, the length of a sequence in one block does not exceed 60 symbols. Optionally, an additional whitespace separated cumulative residue count may follow the sequence symbols. Optionally, a block may be followed by a line depicting the degree of conservation of the respective alignment columns.

Note

Sequence names and the sequences must not contain whitespace characters! Allowed gap symbols are the hyphen ("-"), and dot (".").

Warning

Please note that many programs that output this format tend to truncate the sequence names to a limited number of characters, for instance the first 15 characters. This can destroy the uniqueness of identifiers in your MSA.

Here is an example alignment in ClustalW format:

CLUSTAL W (1.83) multiple sequence alignment

```

AL031296.1/85969-86120      CUGCCUCACAACGUUUGUGCCUCAGUUACCCGUAGAUGUAGUGAGGGUAACAAUACUUAC
AANU01225121.1/438-603      CUGCCUCACAACAUAUUGUGCCUCAGUUACUCAUAGAUGUAGUGAGGGUGACAAUACUUAC
AAWR02037329.1/29294-29150  ---CUCGACACCACU---GCCUCGGUUAACCAUCGGUGCAGUGCGGGUAGUAGUACCAAU

AL031296.1/85969-86120      UCUCGUUGGUGAUAAAGGAACAGCU
AANU01225121.1/438-603      UCUCGUUGGUGAUAAAGGAACAGCU
AAWR02037329.1/29294-29150  GCUAAUUAUUGUGAGGACCAACU

```

8.1.2 Stockholm 1.0 format

Here is an example alignment in Stockholm 1.0 format:

STOCKHOLM 1.0

```

#=GF AC      RF01293
#=GF ID      ACA59
#=GF DE      Small nucleolar RNA ACA59
#=GF AU      Wilkinson A
#=GF SE      Predicted; WAR; Wilkinson A
#=GF SS      Predicted; WAR; Wilkinson A
#=GF GA      43.00
#=GF TC      44.90
#=GF NC      40.30
#=GF TP      Gene; snRNA; snoRNA; HACA-box;
#=GF BM      cmbuild -F CM SEED
#=GF CB      cmcalibrate --mpi CM
#=GF SM      cmsearch --cpu 4 --verbose --nohmmonly -E 1000 -Z 549862.597050 CM SEQDB
#=GF DR      snoRNABase; ACA59;
#=GF DR      SO; 0001263; ncRNA_gene;
#=GF DR      GO; 0006396; RNA processing;
#=GF DR      GO; 0005730; nucleolus;
#=GF RN      [1]
#=GF RM      15199136
#=GF RT      Human box H/ACA pseudouridylation guide RNA machinery.
#=GF RA      Kiss AM, Jady BE, Bertrand E, Kiss T
#=GF RL      Mol Cell Biol. 2004;24:5797-5807.
#=GF WK      Small_nucleolar_RNA
#=GF SQ      3

```

```

AL031296.1/85969-86120      CUGCCUCACAACGUUUGUGCCUCAGUUACCCGUAGAUGUAGUGAGGGUAACAAUACUUACUCUCGUUGGUGAUAAAGGAACAGC
AANU01225121.1/438-603      CUGCCUCACAACAUAUUGUGCCUCAGUUACUCAUAGAUGUAGUGAGGGUGACAAUACUUACUCUCGUUGGUGAUAAAGGAACAGC
AAWR02037329.1/29294-29150  ---CUCGACACCACU---GCCUCGGUUAACCAUCGGUGCAGUGCGGGUAGUAGUACCAUAGCUAAUUAUUGUGAGGACCAAC
#=GC SS_cons      -----(((((, <<<<<<<<_____>>>>>>>>,,,, <<<<<<_____>>>>>>,,,,,))):::~::~:~:
#=GC RF      CUGCcccaCAaCacuuguGCCUCaGUUAaCcCauagguGuAGUGaGgGuggcAaUACccaCcCucgUUgGuggUaAGGAaCAgC
//

```

8.1.3 FASTA (Pearson) format

Note

Sequence names must not contain whitespace characters. Otherwise, the parts after the first whitespace will be dropped. The only allowed gap character is the hyphen ("-").

Here is an example alignment in FASTA format:

```
>AL031296.1/85969-86120
CUGCCUCACAACGUAUUGGCCUCAGUUACCCGUAUGAUGAGGGUAACAAUACUUAC
UCUCGUUGGUGAUAAGGAACAGCU
>AANU01225121.1/438-603
CUGCCUCACAACAUUUGGCCUCAGUUACUCAUAGAUGAUGAGGGUGACAAUACUUAC
UCUCGUUGGUGAUAAGGAACAGCU
>AAWR02037329.1/29294-29150
---CUCGACACCACU---GCCUCGGUUAACCAUCGGUGCAGUGCGGGUAGUAGUACCAAU
GCUAAUUAGUUGAGGACCAACU
```

8.1.4 MAF format

The multiple alignment format (MAF) is usually used to store multiple alignments on DNA level between entire genomes. It consists of independent blocks of aligned sequences which are annotated by their genomic location. Consequently, an MAF formatted MSA file may contain multiple records. MAF files start with a line

```
##maf
```

which is optionally extended by whitespace delimited key=value pairs. Lines starting with the character ("#") are considered comments and usually ignored.

A MAF block starts with character ("a") at the beginning of a line, optionally followed by whitespace delimited key=value pairs. The next lines start with character ("s") and contain sequence information of the form

```
s src start size strand srcSize sequence
```

where

- *src* is the name of the sequence source
- *start* is the start of the aligned region within the source (0-based)
- *size* is the length of the aligned region without gap characters
- *strand* is either ("+") or ("-"), depicting the location of the aligned region relative to the source
- *srcSize* is the size of the entire sequence source, e.g. the full chromosome
- *sequence* is the aligned sequence including gaps depicted by the hyphen ("-")

Here is an example alignment in MAF format (bluntly taken from the [UCSC Genome browser website](#)):

```
##maf version=1 scoring=tba.v8
# tba.v8 ((human chimp) baboon) (mouse rat))
# multiz.v7
# maf_project.v5 _tba_right.maf3 mouse _tba_C
# single_cov2.v4 single_cov2 /dev/stdin

a score=23262.0
s hg16.chr7 27578828 38 + 158545518 AAA-GGGAATGTTAACCAAATGA---ATTGTCTCTTACGGTG
s panTro1.chr6 28741140 38 + 161576975 AAA-GGGAATGTTAACCAAATGA---ATTGTCTCTTACGGTG
s baboon 116834 38 + 4622798 AAA-GGGAATGTTAACCAAATGA---GTTGTCTCTTATGGTG
s mm4.chr6 53215344 38 + 151104725 -AATGGGAATGTTAAGCAAACGA---ATTGTCTCTCAGTGTG
s rn3.chr4 81344243 40 + 187371129 -AA-GGGGATGCTAAGCCAATGAGTTGTTGTCTCTCAATGTG

a score=5062.0
s hg16.chr7 27699739 6 + 158545518 TAAAGA
s panTro1.chr6 28862317 6 + 161576975 TAAAGA
s baboon 241163 6 + 4622798 TAAAGA
s mm4.chr6 53303881 6 + 151104725 TAAAGA
s rn3.chr4 81444246 6 + 187371129 taagga

a score=6636.0
s hg16.chr7 27707221 13 + 158545518 gcagctgaaaaca
s panTro1.chr6 28869787 13 + 161576975 gcagctgaaaaca
s baboon 249182 13 + 4622798 gcagctgaaaaca
s mm4.chr6 53310102 13 + 151104725 ACAGCTGAAAATA
```

8.2 File formats to manipulate the RNA folding grammar

8.2.1 Command Files

The RNAlib and many programs of the ViennaRNA Package can parse and apply data from so-called command files. These commands may refer to structure constraints or even extensions of the RNA folding grammar (such as [Unstructured domains](#)). Commands are given as a line of whitespace delimited data fields. The syntax we use extends the constraint definitions used in the [mfold](#) / [UNAFold](#) software, where each line begins with a command character followed by a set of positions.

However, we introduce several new commands, and allow for an optional loop type context specifier in form of a sequence of characters, and an orientation flag that enables one to force a nucleotide to pair upstream, or downstream.

8.2.1.1 Constraint commands

The following set of commands is recognized:

- F ... Force
- P ... Prohibit
- C ... Conflicts/Context dependency
- A ... Allow (for non-canonical pairs)
- E ... Soft constraints for unpaired position(s), or base pair(s)

8.2.1.2 RNA folding grammar extensions

- UD ... Add ligand binding using the [Unstructured domains](#) feature

8.2.1.3 Specification of the loop type context

The optional loop type context specifier [LOOP] may be a combination of the following:

- E . . . Exterior loop
- H . . . Hairpin loop
- I . . . Interior loop
- M . . . Multibranch loop
- A . . . All loops

For structure constraints, we additionally allow one to address base pairs enclosed by a particular kind of loop, which results in the specifier [WHERE] which consists of [LOOP] plus the following character:

- i . . . enclosed pair of an Interior loop
- m . . . enclosed pair of a Multibranch loop

If no [LOOP] or [WHERE] flags are set, all contexts are considered (equivalent to A)

8.2.1.4 Controlling the orientation of base pairing

For particular nucleotides that are forced to pair, the following [ORIENTATION] flags may be used:

- U . . . Upstream
- D . . . Downstream

If no [ORIENTATION] flag is set, both directions are considered.

8.2.1.5 Sequence coordinates

Sequence positions of nucleotides/base pairs are 1— based and consist of three positions i , j , and k . Alternatively, four positions may be provided as a pair of two position ranges $[i : j]$, and $[k : l]$ using the '-' sign as delimiter within each range, i.e. $i - j$, and $k - l$.

8.2.1.6 Valid constraint commands

Below are resulting general cases that are considered *valid* constraints:

1. "Forcing a range of nucleotide positions to be paired":

Syntax:

```
F i 0 k [WHERE] [ORIENTATION]
```

Description:

Enforces the set of k consecutive nucleotides starting at position i to be paired. The optional loop type specifier [WHERE] allows to force them to appear as closing/enclosed pairs of certain types of loops.

2. "Forcing a set of consecutive base pairs to form":

Syntax:

```
F i j k [WHERE]
```

Description:

Enforces the base pairs $(i, j), \dots, (i + (k - 1), j - (k - 1))$ to form. The optional loop type specifier [WHERE] allows to specify in which loop context the base pair must appear.

3. "Prohibiting a range of nucleotide positions to be paired":

Syntax:

```
P i 0 k [WHERE]
```

Description:

Prohibit a set of k consecutive nucleotides to participate in base pairing, i.e. make these positions unpaired. The optional loop type specifier [WHERE] allows to force the nucleotides to appear within the loop of specific types.

4. "Prohibiting a set of consecutive base pairs to form":

Syntax:

```
P i j k [WHERE]
```

Description:

Prohibit the base pairs $(i, j), \dots, (i + (k - 1), j - (k - 1))$ to form. The optional loop type specifier [WHERE] allows to specify the type of loop they are disallowed to be the closing or an enclosed pair of.

5. "Prohibiting two ranges of nucleotides to pair with each other":

Syntax:

```
P i-j k-l [WHERE]
```

Description:

Prohibit any nucleotide $p \in [i : j]$ to pair with any other nucleotide $q \in [k : l]$. The optional loop type specifier [WHERE] allows to specify the type of loop they are disallowed to be the closing or an enclosed pair of.

6. "Enforce a loop context for a range of nucleotide positions":

Syntax:

```
C i 0 k [WHERE]
```

Description:

This command enforces nucleotides to be unpaired similar to *prohibiting* nucleotides to be paired, as described above. It too marks the corresponding nucleotides to be unpaired, however, the [WHERE] flag can be used to enforce specific loop types the nucleotides must appear in.

7. "Remove pairs that conflict with a set of consecutive base pairs":

Syntax:

C i j k

Description:

Remove all base pairs that conflict with a set of consecutive base pairs $(i, j), \dots, (i + (k - 1), j - (k - 1))$.

Two base pairs (i, j) and (p, q) conflict with each other if $i < p < j < q$, or $p < i < q < j$.

8. "Allow a set of consecutive (non-canonical) base pairs to form":

Syntax:

A i j k [WHERE]

Description:

This command enables the formation of the consecutive base pairs $(i, j), \dots, (i + (k - 1), j - (k - 1))$, no matter if they are *canonical*, or *non-canonical*. In contrast to the above \mathbb{F} and \mathbb{W} commands, which remove conflicting base pairs, the \mathbb{A} command does not. Therefore, it may be used to allow *non-canonical* base pair interactions. Since the RNAlib does not contain free energy contributions E_{ij} for non-canonical base pairs (i, j) , they are scored as the *maximum* of similar, known contributions. In terms of a *Nussinov* like scoring function the free energy of non-canonical base pairs is therefore estimated as

$$E_{ij} = \min \left[\max_{(i,k) \in \{GC, CG, AU, UA, GU, UG\}} E_{ik}, \max_{(k,j) \in \{GC, CG, AU, UA, GU, UG\}} E_{kj} \right].$$

The optional loop type specifier [WHERE] allows to specify in which loop context the base pair may appear.

9. "Apply pseudo free energy to a range of unpaired nucleotide positions":

Syntax:

E i 0 k e

Description:

Use this command to apply a pseudo free energy of e to the set of k consecutive nucleotides, starting at position i . The pseudo free energy is applied only if these nucleotides are considered unpaired in the recursions, or evaluations, and is expected to be given in *kcal/mol*.

10. "Apply pseudo free energy to a set of consecutive base pairs":

Syntax

E i j k e

Use this command to apply a pseudo free energy of e to the set of base pairs $(i, j), \dots, (i + (k - 1), j - (k - 1))$. Energies are expected to be given in *kcal/mol*.

8.2.1.7 Valid domain extensions commands

1. "Add ligand binding to unpaired motif (a.k.a. unstructured domains)":

Syntax:

UD m e [LOOP]

Description:

Add ligand binding to unpaired sequence motif m (given in IUPAC format, capital letters) with binding energy e in particular loop type(s).

Example:

```
UD AAA -5.0 A
```

The above example applies a binding free energy of $-5kcal/mol$ for a motif AAA that may be present in all loop types.

Chapter 9

Examples

9.1 Example programs using the RNAlib C library

9.1.1 Using the 'old' API

The following program exercises most commonly used functions of the library. The program folds two sequences using both the mfe and partition function algorithms and calculates the tree edit and profile distance of the resulting structures and base pairing probabilities.

Note

This program uses the old API of RNAlib, which is in part already marked deprecated. Please consult the [RNAlib API v3.0](#) page for details of what changes are necessary to port your implementation to the new API.

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <string.h>
#include "utils.h"
#include "fold_vars.h"
#include "fold.h"
#include "part_func.h"
#include "inverse.h"
#include "RNAstruct.h"
#include "treedist.h"
#include "stringdist.h"
#include "profiledist.h"

void main()
{
    char *seq1="CGCAGGGGAUACCCGCG", *seq2="GCGCCCAUAGGGACGC",
        *struct1,* struct2,* xstruc;
    float e1, e2, tree_dist, string_dist, profile_dist, kT;
    Tree *T1, *T2;
    swString *S1, *S2;
    float *pf1, *pf2;
    FLT_OR_DBL *bppm;
    /* fold at 30C instead of the default 37C */
    temperature = 30.;          /* must be set *before* initializing */

    /* allocate memory for structure and fold */
    struct1 = (char* ) space(sizeof(char)*(strlen(seq1)+1));
    e1 = fold(seq1, struct1);

    struct2 = (char* ) space(sizeof(char)*(strlen(seq2)+1));
    e2 = fold(seq2, struct2);

    free_arrays();              /* free arrays used in fold() */

    /* produce tree and string representations for comparison */
    xstruc = expand_Full(struct1);
    T1 = make_tree(xstruc);
```

```

S1 = Make_swString(xstruc);
free(xstruc);

xstruc = expand_Full(struct2);
T2 = make_tree(xstruc);
S2 = Make_swString(xstruc);
free(xstruc);

/* calculate tree edit distance and aligned structures with gaps */
edit_backtrack = 1;
tree_dist = tree_edit_distance(T1, T2);
free_tree(T1); free_tree(T2);
unexpand_aligned_F(aligned_line);
printf("%s\n%s  %3.2f\n", aligned_line[0], aligned_line[1], tree_dist);

/* same thing using string edit (alignment) distance */
string_dist = string_edit_distance(S1, S2);
free(S1); free(S2);
printf("%s mfe=%5.2f\n%s mfe=%5.2f dist=%3.2f\n",
       aligned_line[0], e1, aligned_line[1], e2, string_dist);

/* for longer sequences one should also set a scaling factor for
   partition function folding, e.g: */
kT = (temperature+273.15)*1.98717/1000.; /* kT in kcal/mol */
pf_scale = exp(-e1/kT/strlen(seq1));

/* calculate partition function and base pair probabilities */
e1 = pf_fold(seq1, struct1);
/* get the base pair probability matrix for the previous run of pf_fold() */
bppm = export_bppm();
pf1 = Make_bp_profile_bppm(bppm, strlen(seq1));

e2 = pf_fold(seq2, struct2);
/* get the base pair probability matrix for the previous run of pf_fold() */
bppm = export_bppm();
pf2 = Make_bp_profile_bppm(bppm, strlen(seq2));

free_pf_arrays(); /* free space allocated for pf_fold() */

profile_dist = profile_edit_distance(pf1, pf2);
printf("%s free energy=%5.2f\n%s free energy=%5.2f dist=%3.2f\n",
       aligned_line[0], e1, aligned_line[1], e2, profile_dist);

free_profile(pf1); free_profile(pf2);
}

```

In a typical Unix environment you would compile this program using:

```
00001 cc ${OPENMP_CFLAGS} -c example.c -I${hpath}
```

and link using

```
00001 cc ${OPENMP_CFLAGS} -o example -L${lpath} -lRNA -lm
```

where *hpath* and *lpath* point to the location of the header files and library, respectively.

Note

As default, the RNAlib is compiled with build-in *OpenMP* multithreading support. Thus, when linking your own object files to the library you have to pass the compiler specific *OPENMP_CFLAGS* (e.g. '-fopenmp' for **gcc**) even if your code does not use openmp specific code. However, in that case the *OpenMP* flags may be omitted when compiling example.c

9.1.2 Using the 'new' v3.0 API

The following is a simple program that computes the MFE, partition function, and centroid structure by making use of the v3.0 API.

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>

#include <ViennaRNA/data_structures.h>
#include <ViennaRNA/params.h>
#include <ViennaRNA/utils.h>
#include <ViennaRNA/eval.h>
#include <ViennaRNA/fold.h>
#include <ViennaRNA/part_func.h>

int main(int argc, char *argv[]){

    char *seq = "
        AGACGACAAGGUUGAAUCGCACCCACAGUCUAUGAGUCGGUGACAACAUAUACGAAAGGCUGUAAAAUCAUUUAUUCACCACAGGGGGCCCCCGUGUCUAG";
    char *mfe_structure = vrna_alloc(sizeof(char) * (strlen(seq) + 1));
    char *prob_string = vrna_alloc(sizeof(char) * (strlen(seq) + 1));

    /* get a vrna_fold_compound with default settings */
    vrna_fold_compound_t *vc = vrna_fold_compound(seq, NULL,
        VRNA_OPTION_DEFAULT);

    /* call MFE function */
    double mfe = (double)vrna_mfe(vc, mfe_structure);

    printf("%s\n%s (%6.2f)\n", seq, mfe_structure, mfe);

    /* rescale parameters for Boltzmann factors */
    vrna_exp_params_rescale(vc, &mfe);

    /* call PF function */
    FLT_OR_DBL en = vrna_pf(vc, prob_string);

    /* print probability string and free energy of ensemble */
    printf("%s (%6.2f)\n", prob_string, en);

    /* compute centroid structure */
    double dist;
    char *cent = vrna_centroid(vc, &dist);

    /* print centroid structure, its free energy and mean distance to the ensemble */
    printf("%s (%6.2f d=%6.2f)\n", cent, vrna_eval_structure(vc, cent), dist);

    /* free centroid structure */
    free(cent);

    /* free pseudo dot-bracket probability string */
    free(prob_string);

    /* free mfe structure */
    free(mfe_structure);

    /* free memory occupied by vrna_fold_compound */
    vrna_fold_compound_free(vc);

    return EXIT_SUCCESS;
}
```

9.2 Perl Examples

9.2.1 Using the Flat Interface

Example 1: "Simple MFE prediction"

```
00001 #!/usr/bin/perl
00002
00003 use warnings;
00004 use strict;
```

```

00005
00006 use RNA;
00007
00008 my $seq1 = "CGCAGGGAUACCCGCG";
00009
00010 # compute minimum free energy (mfe) and corresponding structure
00011 my ($ss, $mfe) = RNA::fold($seq1);
00012
00013 # print output
00014 printf "%s [ %.2f ]\n", $ss, $mfe;

```

9.2.2 Using the Object Oriented (OO) Interface

The 'fold_compound' class that serves as an object oriented interface for [vrna_fold_compound_t](#)

Example 1: "Simple MFE prediction"

```

00001 #!/usr/bin/perl
00002
00003 use warnings;
00004 use strict;
00005
00006 use RNA;
00007
00008 my $seq1 = "CGCAGGGAUACCCGCG";
00009
00010 # create new fold_compound object
00011 my $fc = new RNA::fold_compound($seq1);
00012
00013 # compute minimum free energy (mfe) and corresponding structure
00014 my ($ss, $mfe) = $fc->mfe();
00015
00016 # print output
00017 printf "%s [ %.2f ]\n", $ss, $mfe;

```

9.3 Python Examples

9.3.1 Using the Flat Interface

Example 1: "Simple MFE prediction"

```

00001 import RNA
00002
00003 sequence = "CUCGUCGCCUUAUCCAGUGCGGGCGCUAGACAUCUAGUUUUCGCCGCAA"
00004
00005 # compute minimum free energy (mfe) and corresponding structure
00006 (structure, mfe) = RNA.fold(sequence)
00007
00008 # print output
00009 print "%s\n%s [ %.2f ]" % (structure, mfe)

```

9.3.2 Using the Object Oriented (OO) Interface

The 'fold_compound' class that serves as an object oriented interface for [vrna_fold_compound_t](#)

Example 1: "Simple MFE prediction"

```

00001 import RNA;
00002
00003 sequence = "CGCAGGGAUACCCGCG"
00004
00005 # create new fold_compound object
00006 fc = RNA.fold_compound(sequence)
00007
00008 # compute minimum free energy (mfe) and corresponding structure
00009 (ss, mfe) = fc.mfe()
00010
00011 # print output
00012 print "%s [ %6.2f ]" % (ss, mfe)

```

Example 2: "Use callback while generating suboptimal structures"

```

00001 import RNA
00002
00003 sequence = "GGGGAAAACCCC"
00004
00005 # Set global switch for unique ML decomposition
00006 RNA.cvar.uniq_ML = 1
00007
00008 subopt_data = { 'counter' : 1, 'sequence' : sequence }
00009
00010 # Print a subopt result as FASTA record
00011 def print_subopt_result(structure, energy, data):
00012     if not structure == None:
00013         print ">subopt %d" % data['counter']
00014         print "%s" % data['sequence']
00015         print "%s [%6.2f]" % (structure, energy)
00016         # increase structure counter
00017         data['counter'] = data['counter'] + 1
00018
00019 # Create a 'fold_compound' for our sequence
00020 a = RNA.fold_compound(sequence)
00021
00022 # Enumerate all structures 500 docal/mol = 5 kcal/mol arround
00023 # the MFE and print each structure using the function above
00024 a.subopt_cb(500, print_subopt_result, subopt_data);

```

Example 3: "Revert MFE to Maximum Matching using soft constraint callbacks"

```

00001 import RNA
00002
00003 seq1 = "CUCGUCGCCUUAUCCAGUGCGGCGCUAGACAUCUAGUUAUCGCCGCAA"
00004
00005 # Turn-off dangles globally
00006 RNA.cvar.dangles = 0
00007
00008 # Data structure that will be passed to our MaximumMatching() callback with two components:
00009 # 1. a 'dummy' fold_compound to evaluate loop energies w/o constraints, 2. a fresh set of energy parameters
00010 mm_data = { 'dummy': RNA.fold_compound(seq1), 'params': RNA.param() }
00011
00012 # Nearest Neighbor Parameter reversal functions
00013 revert_NN = {
00014     RNA.DECOMP_PAIR_HP: lambda i, j, k, l, f, p: - f.eval_hp_loop(i, j) - 100,
00015     RNA.DECOMP_PAIR_IL: lambda i, j, k, l, f, p: - f.eval_int_loop(i, j, k, l) - 100,
00016     RNA.DECOMP_PAIR_ML: lambda i, j, k, l, f, p: - p.MLclosing - p.MLintern[0] - (j - i - k + 1 - 2)
00017     * p.MLbase - 100,
00018     RNA.DECOMP_ML_ML_STEM: lambda i, j, k, l, f, p: - p.MLintern[0] - (l - k - 1) * p.MLbase,
00019     RNA.DECOMP_ML_IL: lambda i, j, k, l, f, p: - p.MLintern[0] - (j - i - k + 1) * p.MLbase,
00020     RNA.DECOMP_ML_ML: lambda i, j, k, l, f, p: - (j - i - k + 1) * p.MLbase,
00021     RNA.DECOMP_ML_UP: lambda i, j, k, l, f, p: - (j - i + 1) * p.MLbase,
00022     RNA.DECOMP_EXT_STEM: lambda i, j, k, l, f, p: - f.E_ext_loop(k, l),
00023     RNA.DECOMP_EXT_STEM_EXT: lambda i, j, k, l, f, p: - f.E_ext_loop(i, k),
00024     RNA.DECOMP_EXT_EXT_STEM: lambda i, j, k, l, f, p: - f.E_ext_loop(l, j),
00025     RNA.DECOMP_EXT_EXT_STEM1: lambda i, j, k, l, f, p: - f.E_ext_loop(l, j-1),
00026 }
00027
00027 # Maximum Matching callback function (will be called by RNAlib in each decomposition step)
00028 def MaximumMatching(i, j, k, l, d, data):
00029     return revert_NN[d](i, j, k, l, data['dummy'], data['params'])
00030
00031 # Create a 'fold_compound' for our sequence
00032 fc = RNA.fold_compound(seq1)
00033
00034 # Add maximum matching soft-constraints
00035 fc.sc_add_f(MaximumMatching)
00036 fc.sc_add_data(mm_data, None)
00037

```

```
00038 # Call MFE algorithm
00039 (s, mm) = fc.mfe()
00040
00041 # print result
00042 print "%s\n%s (MM: %d)\n" % (seq1, s, -mm)
00043
```

Chapter 10

Deprecated List

Global **alifold** (const char **strings, char *structure)

Usage of this function is discouraged! Use [vrna_alifold\(\)](#), or [vrna_mfe\(\)](#) instead!

Global **alimake_pair_table** (const char *structure)

Use [vrna_pt_ali_get\(\)](#) instead!

Global **alipbacktrack** (double *prob)

Use [vrna_pbacktrack\(\)](#) instead!

Global **alipf_circ_fold** (const char **sequences, char *structure, vrna_plist_t **pl)

Use [vrna_pf\(\)](#) instead

Global **alipf_fold** (const char **sequences, char *structure, vrna_plist_t **pl)

Use [vrna_pf\(\)](#) instead

Global **alipf_fold_par** (const char **sequences, char *structure, vrna_plist_t **pl, vrna_exp_param_t *parameters, int calculate_bppm, int is_constrained, int is_circular)

Use [vrna_pf\(\)](#) instead

Global **assign_plist_from_db** (vrna_plist_t **pl, const char *struc, float pr)

Use [vrna_plist\(\)](#) instead

Global **assign_plist_from_pr** (vrna_plist_t **pl, FLT_OR_DBL *probs, int length, double cutoff)

Use [vrna_plist_from_probs\(\)](#) instead!

Global **base_pair**

Do not use this variable anymore!

Global **bondT**

Use [vrna_bp_stack_t](#) instead!

Global **bp_distance** (const char *str1, const char *str2)

Use [vrna_bp_distance](#) instead

Global **bppm_symbol** (const float *x)

Use [vrna_bpp_symbol\(\)](#) instead!

Global **bppm_to_structure** (char *structure, FLT_OR_DBL *pr, unsigned int length)

Use [vrna_db_from_probs\(\)](#) instead!

Global **centroid** (int length, double *dist)

This function is deprecated and should not be used anymore as it is not threadsafe!

Global **circalifold** (const char **strings, char *structure)

Usage of this function is discouraged! Use [vrna_alicircfold\(\)](#), and [vrna_mfe\(\)](#) instead!

Global **circfold** (const char *sequence, char *structure)

Use [vrna_circfold\(\)](#), or [vrna_mfe\(\)](#) instead!

Global **co_pf_fold** (char *sequence, char *structure)

{Use [vrna_pf_dimer\(\)](#) instead!}

Global **co_pf_fold_par** (char *sequence, char *structure, vrna_exp_param_t *parameters, int calculate_bpmm, int is_constrained)

Use [vrna_pf_dimer\(\)](#) instead!

Global **cofold** (const char *sequence, char *structure)

use [vrna_mfe_dimer\(\)](#) instead

Global **cofold_par** (const char *string, char *structure, vrna_param_t *parameters, int is_constrained)

use [vrna_mfe_dimer\(\)](#) instead

Global **compute_BPdifferences** (short *pt1, short *pt2, unsigned int turn)

Use [vrna_refBPdist_matrix\(\)](#) instead

Global **compute_probabilities** (double FAB, double FEA, double FEB, vrna_plist_t *prAB, vrna_plist_t *prA, vrna_plist_t *prB, int Alength)

{ Use [vrna_pf_dimer_probs\(\)](#) instead!}

Global **constrain_ptypes** (const char *constraint, unsigned int length, char *ptype, int *BP, int min_loop_size, unsigned int idx_type)

Do not use this function anymore! Structure constraints are now handled through [vrna_hc_t](#) and related functions.

Global **copy_pair_table** (const short *pt)

Use [vrna_ptable_copy\(\)](#) instead

Global **cpair**

Use [vrna_cpair_t](#) instead!

Global **cv_fact**

See [vrna_md_t.cv_fact](#), and [vrna_mfe\(\)](#) to avoid using global variables

Global **destroy_TwoDfold_variables** (TwoDfold_vars *our_variables)

Use the new API that relies on [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_mfe_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Global **destroy_TwoDpfold_variables** (TwoDpfold_vars *vars)

Use the new API that relies on [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_pf_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Global **energy_of_alistruct** (const char **sequences, const char *structure, int n_seq, float *energy)

Usage of this function is discouraged! Use [vrna_eval_structure\(\)](#), and [vrna_eval_covar_structure\(\)](#) instead!

Global **energy_of_circ_struct** (const char *string, const char *structure)

This function is deprecated and should not be used in future programs Use [energy_of_circ_structure\(\)](#) instead!

Global **energy_of_circ_struct_par** (const char *string, const char *structure, vrna_param_t *parameters, int verbosity_level)

Use [vrna_eval_structure\(\)](#) or [vrna_eval_structure_verbose\(\)](#) instead!

Global **energy_of_circ_structure** (const char *string, const char *structure, int verbosity_level)

Use [vrna_eval_structure\(\)](#) or [vrna_eval_structure_verbose\(\)](#) instead!

Global **energy_of_move** (const char *string, const char *structure, int m1, int m2)

Use [vrna_eval_move\(\)](#) instead!

Global **energy_of_move_pt** (short *pt, short *s, short *s1, int m1, int m2)

Use [vrna_eval_move_pt\(\)](#) instead!

Global **energy_of_struct** (const char *string, const char *structure)

This function is deprecated and should not be used in future programs! Use [energy_of_structure\(\)](#) instead!

Global **energy_of_struct_par** (const char *string, const char *structure, vrna_param_t *parameters, int verbosity_level)

Use [vrna_eval_structure\(\)](#) or [vrna_eval_structure_verbose\(\)](#) instead!

Global **energy_of_struct_pt** (const char *string, short *ptable, short *s, short *s1)

This function is deprecated and should not be used in future programs! Use [energy_of_structure_pt\(\)](#) instead!

Global **energy_of_struct_pt_par** (const char *string, short *ptable, short *s, short *s1, vrna_param_t *parameters, int verbosity_level)

Use [vrna_eval_structure_pt\(\)](#) or [vrna_eval_structure_pt_verbose\(\)](#) instead!

Global **energy_of_structure** (const char *string, const char *structure, int verbosity_level)

Use [vrna_eval_structure\(\)](#) or [vrna_eval_structure_verbose\(\)](#) instead!

Global **energy_of_structure_pt** (const char *string, short *ptable, short *s, short *s1, int verbosity_level)

Use [vrna_eval_structure_pt\(\)](#) or [vrna_eval_structure_pt_verbose\(\)](#) instead!

Global **expHairpinEnergy** (int u, int type, short si1, short sj1, const char *string)

Use [exp_E_Hairpin\(\)](#) from [loop_energies.h](#) instead

Global **expLoopEnergy** (int u1, int u2, int type, int type2, short si1, short sj1, short sp1, short sq1)

Use [exp_E_IntLoop\(\)](#) from [loop_energies.h](#) instead

Global **export_ali_bppm** (void)

Usage of this function is discouraged! The new [vrna_fold_compound_t](#) allows direct access to the folding matrices, including the pair probabilities! The pair probability array returned here reflects the one of the latest call to [vrna_pf\(\)](#), or any of the old API calls for consensus structure partition function folding.

Global **export_circfold_arrays** (int *Fc_p, int *FcH_p, int *FcI_p, int *FcM_p, int **fM2_p, int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **indx_p, char **ptype_p)

See [vrna_mfe\(\)](#) and [vrna_fold_compound_t](#) for the usage of the new API!

Global **export_circfold_arrays_par** (int *Fc_p, int *FcH_p, int *FcI_p, int *FcM_p, int **fM2_p, int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **indx_p, char **ptype_p, vrna_param_t **P_p)

See [vrna_mfe\(\)](#) and [vrna_fold_compound_t](#) for the usage of the new API!

Global **export_co_bppm** (void)

This function is deprecated and will be removed soon! The base pair probability array is available through the [vrna_fold_compound_t](#) data structure, and its associated [vrna_mx_pf_t](#) member.

Global **export_cofold_arrays** (int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **fc_p, int **indx_p, char **ptype_p)

folding matrices now reside within the [vrna_fold_compound_t](#). Thus, this function will only work in conjunction with a prior call to the deprecated functions [cofold\(\)](#) or [cofold_par\(\)](#)

Global **export_cofold_arrays_gg** (int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **fc_p, int **ggg_p, int **indx_p, char **ptype_p)

folding matrices now reside within the fold compound. Thus, this function will only work in conjunction with a prior call to [cofold\(\)](#) or [cofold_par\(\)](#)

Global **export_fold_arrays** (int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **indx_p, char **ptype_p)

See [vrna_mfe\(\)](#) and [vrna_fold_compound_t](#) for the usage of the new API!

Global **export_fold_arrays_par** (int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **indx_p, char **ptype_p, vrna_param_t **P_p)

See [vrna_mfe\(\)](#) and [vrna_fold_compound_t](#) for the usage of the new API!

Global **filecopy** (FILE *from, FILE *to)

Use [vrna_file_copy\(\)](#) instead!

Global **fold** (const char *sequence, char *structure)

use [vrna_fold\(\)](#), or [vrna_mfe\(\)](#) instead!

Global **fold_par** (const char *sequence, char *structure, vrna_param_t *parameters, int is_constrained, int is_circular)

use [vrna_mfe\(\)](#) instead!

Global **free_alifold_arrays** (void)

Usage of this function is discouraged! It only affects memory being free'd that was allocated by an old API function before. Release of memory occupied by the newly introduced [vrna_fold_compound_t](#) is handled by [vrna_vrna_fold_compound_free\(\)](#)

Global **free_alipf_arrays** (void)

Usage of this function is discouraged! This function only free's memory allocated by old API function calls. Memory allocated by any of the new API calls (starting with vrna_) will be not affected!

Global **free_arrays** (void)

See [vrna_fold\(\)](#), [vrna_circfold\(\)](#), or [vrna_mfe\(\)](#) and [vrna_fold_compound_t](#) for the usage of the new API!

Global **free_co_arrays** (void)

This function will only free memory allocated by a prior call of [cofold\(\)](#) or [cofold_par\(\)](#). See [vrna_mfe_dimer\(\)](#) for how to use the new API

Global **free_co_pf_arrays** (void)

This function will be removed for the new API soon! See [vrna_pf_dimer\(\)](#), [vrna_fold_compound\(\)](#), and [vrna_fold_compound_free\(\)](#) for an alternative

Global **free_pf_arrays** (void)

See [vrna_fold_compound_t](#) and its related functions for how to free memory occupied by the dynamic programming matrices

Global **get_alipf_arrays** (short ***S_p, short ***S5_p, short ***S3_p, unsigned short ***a2s_p, char ***Ss_p, FLT_OR_DBL **qb_p, FLT_OR_DBL **qm_p, FLT_OR_DBL **q1k_p, FLT_OR_DBL **qln_p, short **pscore)

It is discouraged to use this function! The new [vrna_fold_compound_t](#) allows direct access to all necessary consensus structure prediction related variables!

Global **get_boltzmann_factor_copy** (vrna_exp_param_t *parameters)

Use [vrna_exp_params_copy\(\)](#) instead!

Global **get_boltzmann_factors** (double temperature, double betaScale, vrna_md_t md, double pf_scale)

Use [vrna_exp_params\(\)](#) instead!

Global **get_boltzmann_factors_ali** (unsigned int n_seq, double temperature, double betaScale, vrna_md_t md, double pf_scale)

Use [vrna_exp_params_comparative\(\)](#) instead!

Global **get_centroid_struct_gquad_pr** (int length, double *dist)

This function is deprecated and should not be used anymore as it is not threadsafe!

Global **get_centroid_struct_pl** (int length, double *dist, vrna_plist_t *pl)

This function was renamed to [vrna_centroid_from_plist\(\)](#)

Global **get_centroid_struct_pr** (int length, double *dist, FLT_OR_DBL *pr)

This function was renamed to [vrna_centroid_from_probs\(\)](#)

Global **get_concentrations** (double FEAB, double FEAA, double FEBB, double FEA, double FEB, double *startconc)

{ Use [vrna_pf_dimer_concentrations\(\)](#) instead! }

Global **get_line** (FILE *fp)

Use [vrna_read_line\(\)](#) as a substitute!

Global **get_monomere_mfes** (float *e1, float *e2)

{This function is obsolete and will be removed soon!}

Global **get_mpi** (char *Alseq[], int n_seq, int length, int *mini)

Use [vrna_aln_mpi\(\)](#) as a replacement

Global **get_plist** (vrna_plist_t *pl, int length, double cut_off)

{ This function is deprecated and will be removed soon!} use [assign_plist_from_pr\(\)](#) instead!

Global **get_scaled_alipf_parameters** (unsigned int n_seq)

Use [vrna_exp_params_comparative\(\)](#) instead!

Global **get_scaled_parameters** (double temperature, vrna_md_t md)

Use [vrna_params\(\)](#) instead!

Global **get_scaled_pf_parameters** (void)

Use [vrna_exp_params\(\)](#) instead!

Global **get_TwoDfold_variables** (const char *seq, const char *structure1, const char *structure2, int circ)

Use the new API that relies on [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound↵_TwoD\(\)](#), [vrna_mfe_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Global **get_TwoDpfold_variables** (const char *seq, const char *structure1, char *structure2, int circ)

Use the new API that relies on [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound↵_TwoD\(\)](#), [vrna_pf_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Global **HairpinE** (int size, int type, int si1, int sj1, const char *string)

{This function is deprecated and will be removed soon. Use [E_Hairpin\(\)](#) instead!}

Global **hamming** (const char *s1, const char *s2)

Use [vrna_hamming_distance\(\)](#) instead!

Global **hamming_bound** (const char *s1, const char *s2, int n)

Use [vrna_hamming_distance_bound\(\)](#) instead!

Global **iindx**

Do not use this variable anymore!

Global **init_co_pf_fold** (int length)

{ This function is deprecated and will be removed soon!}

Global **init_pf_fold** (int length)

This function is obsolete and will be removed soon!

Global **init_rand** (void)

Use [vrna_init_rand\(\)](#) instead!

Global **initialize_cofold** (int length)

{This function is obsolete and will be removed soon!}

Global **initialize_fold** (int length)

See [vrna_mfe\(\)](#) and [vrna_fold_compound_t](#) for the usage of the new API!

Global **int_urn** (int from, int to)

Use [vrna_int_urn\(\)](#) instead!

Global **Lfold** (const char *string, char *structure, int maxdist)

Use [vrna_mfe_window\(\)](#) instead!

Global **Lfoldz** (const char *string, char *structure, int maxdist, int zsc, double min_z)

Use [vrna_mfe_window_zscore\(\)](#) instead!

Global **loop_energy** (short *ptable, short *s, short *s1, int i)

Use [vrna_eval_loop_pt\(\)](#) instead!

Global **LoopEnergy** (int n1, int n2, int type, int type_2, int si1, int sj1, int sp1, int sq1)

{This function is deprecated and will be removed soon. Use [E_IntLoop\(\)](#) instead!}

Global **Make_bp_profile** (int length)

This function is deprecated and will be removed soon! See [Make_bp_profile_bppm\(\)](#) for a replacement

Global **make_pair_table** (const char *structure)

Use [vrna_ptable\(\)](#) instead

Global **make_pair_table_snoop** (const char *structure)

Use [vrna_pt_snoop_get\(\)](#) instead!

Global **make_referenceBP_array** (short *reference_pt, unsigned int turn)

Use [vrna_refBPcnt_matrix\(\)](#) instead

Global **mean_bp_dist** (int length)

This function is not threadsafe and should not be used anymore. Use [mean_bp_distance\(\)](#) instead!

Global **mean_bp_distance** (int length)

Use [vrna_mean_bp_distance\(\)](#) or [vrna_mean_bp_distance_pr\(\)](#) instead!

Global **mean_bp_distance_pr** (int length, FLT_OR_DBL *pr)

Use [vrna_mean_bp_distance\(\)](#) or [vrna_mean_bp_distance_pr\(\)](#) instead!

Global **nc_fact**

See [vrna_md_t.nc_fact](#), and [vrna_mfe\(\)](#) to avoid using global variables

Global **nrerror** (const char message[])

Use [vrna_message_error\(\)](#) instead!

Global **pack_structure** (const char *struc)

Use [vrna_db_pack\(\)](#) as a replacement

Global **PAIR**

Use [vrna_basepair_t](#) instead!

Global **pair_info**

Use [vrna_pinfo_t](#) instead!

Global **paramT**

Use [vrna_param_t](#) instead!

Global **parenthesis_structure** (char *structure, vrna_bp_stack_t *bp, int length)

use [vrna_parenthesis_structure\(\)](#) instead

Global **parenthesis_zuker** (char *structure, vrna_bp_stack_t *bp, int length)

use [vrna_parenthesis_zuker](#) instead

Global **path_t**

Use [vrna_path_t](#) instead!

Global **pbacktrack_circ** (char *sequence)

Use [vrna_pbacktrack\(\)](#) instead.

Global **pf_circ_fold** (const char *sequence, char *structure)

Use [vrna_pf\(\)](#) instead!

Global **pf_fold_par** (const char *sequence, char *structure, vrna_exp_param_t *parameters, int calculate_bp, int is_constrained, int is_circular)

Use [vrna_pf\(\)](#) instead

Global **pf_paramT**

Use [vrna_exp_param_t](#) instead!

Global **plist**

Use [vrna_plist_t](#) instead!

Global **pr**

Do not use this variable anymore!

Global **print_tty_constraint** (unsigned int option)

Use [vrna_message_constraints\(\)](#) instead!

Global `print_tty_constraint_full` (void)

Use `vrna_message_constraint_options_all()` instead!

Global `print_tty_input_seq` (void)

Use `vrna_message_input_seq_simple()` instead!

Global `print_tty_input_seq_str` (const char *s)

Use `vrna_message_input_seq()` instead!

Global `PS_dot_plot` (char *string, char *file)

This function is deprecated and will be removed soon! Use `PS_dot_plot_list()` instead!

Global `PS_rna_plot` (char *string, char *structure, char *file)

Use `vrna_file_PS_rnaplot()` instead!

Global `PS_rna_plot_a` (char *string, char *structure, char *file, char *pre, char *post)

Use `vrna_file_PS_rnaplot_a()` instead!

Global `PS_rna_plot_a_gquad` (char *string, char *structure, char *ssfile, char *pre, char *post)

Use `vrna_file_PS_rnaplot_a()` instead!

Global `random_string` (int l, const char symbols[])

Use `vrna_random_string()` instead!

Global `read_record` (char **header, char **sequence, char *rest, unsigned int options)**

This function is deprecated! Use `vrna_file_fasta_read_record()` as a replacement.

Global `scale_parameters` (void)

Use `vrna_params()` instead!

Global `sect`

Use `vrna_sect_t` instead!

Global `set_model_details` (vrna_md_t *md)

This function will vanish as soon as backward compatibility of RNAlib is dropped (expected in version 3). Use `vrna_md_set_default()` instead!

Global `SOLUTION`

Use `vrna_subopt_solution_t` instead!

Global `space` (unsigned size)

Use `vrna_alloc()` instead!

Global `st_back`

set the `uniq_ML` flag in `vrna_md_t` before passing it to `vrna_fold_compound()`.

Global `stackProb` (double cutoff)

Use `vrna_stack_prob()` instead!

Global `str_DNA2RNA` (char *sequence)

Use `vrna_seq_toRNA()` instead!

Global `str_uppercase` (char *sequence)

Use `vrna_seq_toupper()` instead!

Global `temperature`

Use `vrna_md_defaults_temperature()`, and `vrna_md_defaults_temperature_get()` to change, and read the global default temperature settings

Global `time_stamp` (void)

Use `vrna_time_stamp()` instead!

Global `TwoDfold_backtrack_f5` (unsigned int j, int k, int l, `TwoDfold_vars` *vars)

Use the new API that relies on `vrna_fold_compound_t` and the corresponding functions `vrna_fold_compound`↵
_TwoD(), `vrna_mfe_TwoD()`, `vrna_backtrack5_TwoD()`, and `vrna_fold_compound_free()` instead!

Global [TwoDfold_vars](#)

This data structure will be removed from the library soon! Use [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_mfe_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Global [TwoDfoldList](#) ([TwoDfold_vars](#) *vars, int distance1, int distance2)

Use the new API that relies on [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_mfe_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Global [TwoDpfold_pbacktrack](#) ([TwoDpfold_vars](#) *vars, int d1, int d2)

Use the new API that relies on [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_pf_TwoD\(\)](#), [vrna_pbacktrack_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Global [TwoDpfold_pbacktrack5](#) ([TwoDpfold_vars](#) *vars, int d1, int d2, unsigned int length)

Use the new API that relies on [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_pf_TwoD\(\)](#), [vrna_pbacktrack5_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Class [TwoDpfold_vars](#)

This data structure will be removed from the library soon! Use [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_pf_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Global [TwoDpfoldList](#) ([TwoDpfold_vars](#) *vars, int maxDistance1, int maxDistance2)

Use the new API that relies on [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_pf_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Global [unpack_structure](#) (const char *packed)

Use [vrna_db_unpack\(\)](#) as a replacement

Global [update_alifold_params](#) (void)

Usage of this function is discouraged! The new API uses [vrna_fold_compound_t](#) to lump all folding related necessities together, including the energy parameters. Use [vrna_update_fold_params\(\)](#) to update the energy parameters within a [vrna_fold_compound_t](#).

Global [update_co_pf_params](#) (int length)

Use [vrna_exp_params_subst\(\)](#) instead!

Global [update_co_pf_params_par](#) (int length, [vrna_exp_param_t](#) *parameters)

Use [vrna_exp_params_subst\(\)](#) instead!

Global [update_cofold_params](#) (void)

See [vrna_params_subst\(\)](#) for an alternative using the new API

Global [update_cofold_params_par](#) ([vrna_param_t](#) *parameters)

See [vrna_params_subst\(\)](#) for an alternative using the new API

Global [update_fold_params](#) (void)

For non-default model settings use the new API with [vrna_params_subst\(\)](#) and [vrna_mfe\(\)](#) instead!

Global [update_fold_params_par](#) ([vrna_param_t](#) *parameters)

For non-default model settings use the new API with [vrna_params_subst\(\)](#) and [vrna_mfe\(\)](#) instead!

Global [update_pf_params](#) (int length)

Use [vrna_exp_params_subst\(\)](#) instead

Global [update_pf_params_par](#) (int length, [vrna_exp_param_t](#) *parameters)

Use [vrna_exp_params_subst\(\)](#) instead

Global [urn](#) (void)

Use [vrna_urn\(\)](#) instead!

Global [VRNA_CONSTRAINT_FILE](#)

Use 0 instead!

Global [VRNA_CONSTRAINT_MULTILINE](#)

see [vrna_extract_record_rest_structure\(\)](#)

Global `VRNA_CONSTRAINT_NO_HEADER`

This mode is not supported anymore!

Global `VRNA_CONSTRAINT_SOFT_MFE`

This flag has no meaning anymore, since constraints are now always stored!

Global `VRNA_CONSTRAINT_SOFT_PF`

Use `VRNA_OPTION_PF` instead!

Global `vrna_exp_param_s::id`

This attribute will be removed in version 3

Global `vrna_extract_record_rest_constraint` (`char **cstruc, const char **lines, unsigned int option`)

Use `vrna_extract_record_rest_structure()` instead!

Global `vrna_fc_s::pscore_pf_compat`

This attribute will vanish in the future!

Global `vrna_fc_s::ptype_pf_compat`

This attribute will vanish in the future! It's meant for backward compatibility only!

Global `warn_user` (`const char message[]`)

Use `vrna_message_warning()` instead!

Global `xrealloc` (`void *p, unsigned size`)

Use `vrna_realloc()` instead!

Global `zukersubopt` (`const char *string`)

use `vrna_zukersubopt()` instead

Global `zukersubopt_par` (`const char *string, vrna_param_t *parameters`)

use `vrna_zukersubopt()` instead

Chapter 11

Bug List

Module [domains_up](#)

Although the additional production rule(s) for unstructured domains in the descriptions of this feature are always treated as 'segments possibly bound to one or more ligands', the current implementation requires that at least one ligand is bound. The default implementation already takes care of the required changes, however, upon using callback functions other than the default ones, one has to take care of this fact. Please also note, that this behavior might change in one of the next releases, such that the decomposition schemes as shown above comply with the actual implementation.

Global [vrna_subopt_zuker](#) ([vrna_fold_compound_t](#) *vc)

Due to resizing, any pre-existing constraints will be lost!

Chapter 12

Module Index

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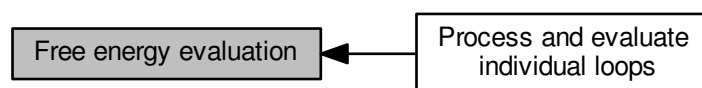
Chapter 15

Module Documentation

15.1 Free energy evaluation

Secondary structure and loop free energy evaluation.

Collaboration diagram for Free energy evaluation:



Modules

- [Process and evaluate individual loops](#)

Files

- file [eval.h](#)

Functions and variables related to energy evaluation of sequence/structure pairs.

Functions

- float [vrna_eval_structure](#) ([vrna_fold_compound_t](#) *vc, const char *structure)
Calculate the free energy of an already folded RNA.
- float [vrna_eval_covar_structure](#) ([vrna_fold_compound_t](#) *vc, const char *structure)
Calculate the pseudo energy derived by the covariance scores of a set of aligned sequences.
- float [vrna_eval_structure_simple](#) (const char *string, const char *structure)
Calculate the free energy of an already folded RNA.

- float [vrna_eval_structure_verbose](#) ([vrna_fold_compound_t](#) *vc, const char *structure, FILE *file)
Calculate the free energy of an already folded RNA and print contributions on a per-loop base.
- float [vrna_eval_structure_v](#) ([vrna_fold_compound_t](#) *vc, const char *structure, int verbosity_level, FILE *file)
Calculate the free energy of an already folded RNA and print contributions on a per-loop base.
- float [vrna_eval_structure_simple_verbose](#) (const char *string, const char *structure, FILE *file)
Calculate the free energy of an already folded RNA and print contributions per loop.
- float [vrna_eval_structure_simple_v](#) (const char *string, const char *structure, int verbosity_level, FILE *file)
Calculate the free energy of an already folded RNA and print contributions per loop.
- int [vrna_eval_structure_pt](#) ([vrna_fold_compound_t](#) *vc, const short *pt)
Calculate the free energy of an already folded RNA.
- int [vrna_eval_structure_pt_simple](#) (const char *string, const short *pt)
Calculate the free energy of an already folded RNA.
- int [vrna_eval_structure_pt_verbose](#) ([vrna_fold_compound_t](#) *vc, const short *pt, FILE *file)
Calculate the free energy of an already folded RNA.
- int [vrna_eval_structure_pt_v](#) ([vrna_fold_compound_t](#) *vc, const short *pt, int verbosity_level, FILE *file)
Calculate the free energy of an already folded RNA.
- int [vrna_eval_structure_pt_simple_verbose](#) (const char *string, const short *pt, FILE *file)
Calculate the free energy of an already folded RNA.
- int [vrna_eval_structure_pt_simple_v](#) (const char *string, const short *pt, int verbosity_level, FILE *file)
Calculate the free energy of an already folded RNA.
- int [vrna_eval_loop_pt](#) ([vrna_fold_compound_t](#) *vc, int i, const short *pt)
Calculate energy of a loop.
- float [vrna_eval_move](#) ([vrna_fold_compound_t](#) *vc, const char *structure, int m1, int m2)
Calculate energy of a move (closing or opening of a base pair)
- int [vrna_eval_move_pt](#) ([vrna_fold_compound_t](#) *vc, short *pt, int m1, int m2)
Calculate energy of a move (closing or opening of a base pair)
- float [energy_of_structure](#) (const char *string, const char *structure, int verbosity_level)
Calculate the free energy of an already folded RNA using global model detail settings.
- float [energy_of_struct_par](#) (const char *string, const char *structure, [vrna_param_t](#) *parameters, int verbosity_level)
Calculate the free energy of an already folded RNA.
- float [energy_of_circ_structure](#) (const char *string, const char *structure, int verbosity_level)
Calculate the free energy of an already folded circular RNA.
- float [energy_of_circ_struct_par](#) (const char *string, const char *structure, [vrna_param_t](#) *parameters, int verbosity_level)
Calculate the free energy of an already folded circular RNA.
- int [energy_of_structure_pt](#) (const char *string, short *ptable, short *s, short *s1, int verbosity_level)
Calculate the free energy of an already folded RNA.
- int [energy_of_struct_pt_par](#) (const char *string, short *ptable, short *s, short *s1, [vrna_param_t](#) *parameters, int verbosity_level)
Calculate the free energy of an already folded RNA.
- float [energy_of_move](#) (const char *string, const char *structure, int m1, int m2)
Calculate energy of a move (closing or opening of a base pair)
- int [energy_of_move_pt](#) (short *pt, short *s, short *s1, int m1, int m2)
Calculate energy of a move (closing or opening of a base pair)
- int [loop_energy](#) (short *ptable, short *s, short *s1, int i)
Calculate energy of a loop.
- float [energy_of_struct](#) (const char *string, const char *structure)
- int [energy_of_struct_pt](#) (const char *string, short *ptable, short *s, short *s1)
- float [energy_of_circ_struct](#) (const char *string, const char *structure)

Variables

- int `cut_point`
set to first pos of second seq for cofolding
- int `eos_debug`
verbose info from energy_of_struct

15.1.1 Detailed Description

Secondary structure and loop free energy evaluation.

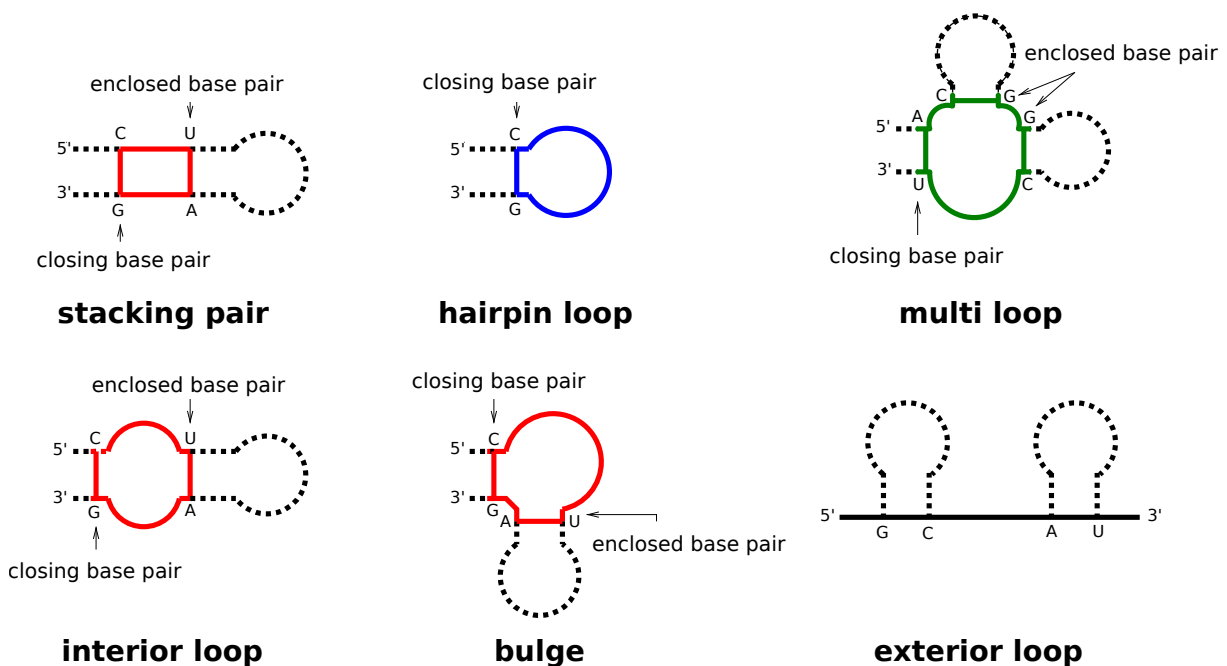
Functions and variables related to free energy evaluation of sequence/structure pairs.

This module covers the functions to evaluate the free energy of a secondary structure given its sequence.

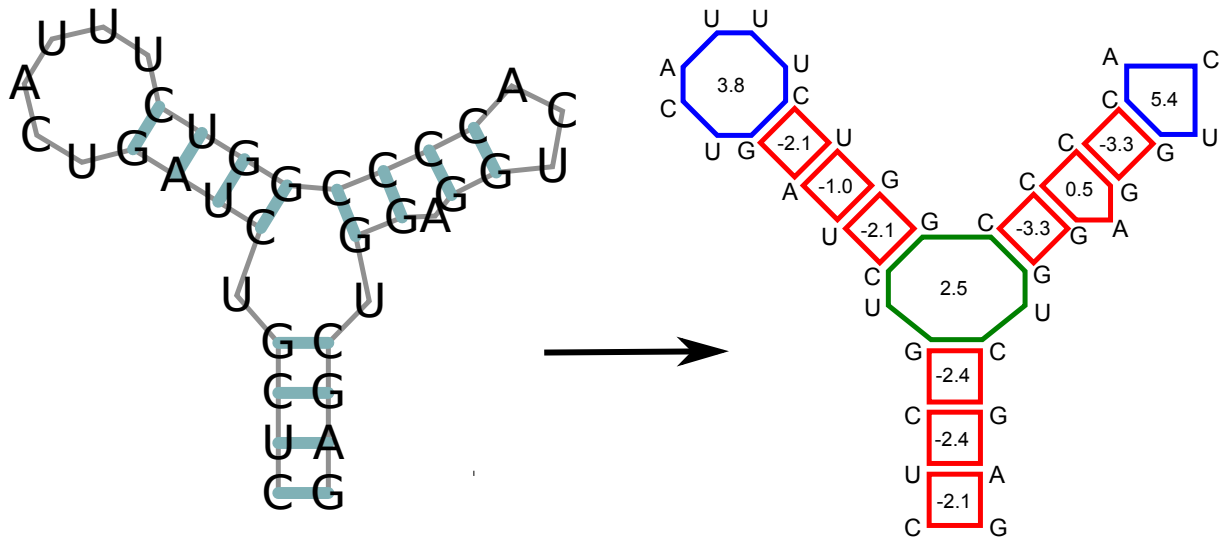
Each base pair in a secondary structure closes a loop, thereby directly enclosing unpaired nucleotides, and/or further base pairs. Our implementation distinguishes four basic types of loops:

- hairpin loops
- interior loops
- multibranch loops
- exterior loop

While the exterior loop is a special case without a closing pair, the other loops are determined by the number of base pairs involved in the loop formation, i.e. hairpin loops are 1-loops, since only a single base pair delimits the loop. interior loops are 2-loops due to their enclosing, and enclosed base pair. All loops where more than two base pairs are involved, are termed multibranch loops.



Any secondary structure can be decomposed into its loops. Each of the loops then can be scored in terms of free energy, and the free energy of an entire secondary structure is simply the sum of free energies of its loops.



15.1.2 Function Documentation

15.1.2.1 `float vrna_eval_structure (vrna_fold_compound_t * vc, const char * structure)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA.

This function allows for energy evaluation of a given pair of structure and sequence (alignment). Model details, energy parameters, and possibly soft constraints are used as provided via the parameter 'vc'. The `vrna_fold_compound_t` does not need to contain any DP matrices, but requires all most basic init values as one would get from a call like this:

```
vc = vrna_fold_compound(sequence, NULL, VRNA_OPTION_EVAL_ONLY);
```

Note

Accepts `vrna_fold_compound_t` of type `VRNA_FC_TYPE_SINGLE` and `VRNA_FC_TYPE_COMPARATIVE`

See also

`vrna_eval_structure_pt()`, `vrna_eval_structure_verbose()`, `vrna_eval_structure_pt_verbose()`, `vrna_fold_compound()`, `vrna_fold_compound_comparative()`, `vrna_eval_covar_structure()`

Parameters

<code>vc</code>	A <code>vrna_fold_compound_t</code> containing the energy parameters and model details
<code>structure</code>	Secondary structure in dot-bracket notation

Returns

The free energy of the input structure given the input sequence in kcal/mol

SWIG Wrapper Notes This function is attached as method `eval_structure()` to objects of type `fold_compound`

15.1.2.2 float vrna_eval_covar_structure (vrna_fold_compound_t * vc, const char * structure)

```
#include <ViennaRNA/eval.h>
```

Calculate the pseudo energy derived by the covariance scores of a set of aligned sequences.

Consensus structure prediction is driven by covariance scores of base pairs in rows of the provided alignment. This function allows one to retrieve the total amount of this covariance pseudo energy scores. The `vrna_fold_compound_t` does not need to contain any DP matrices, but requires all most basic init values as one would get from a call like this:

```
vc = vrna_fold_compound_comparative(alignment, NULL,
    VRNA_OPTION_EVAL_ONLY);
```

Note

Accepts `vrna_fold_compound_t` of type `VRNA_FC_TYPE_COMPARATIVE` only!

See also

[vrna_fold_compound_comparative\(\)](#), [vrna_eval_structure\(\)](#)

Parameters

<i>vc</i>	A <code>vrna_fold_compound_t</code> containing the energy parameters and model details
<i>structure</i>	Secondary (consensus) structure in dot-bracket notation

Returns

The covariance pseudo energy score of the input structure given the input sequence alignment in kcal/mol

SWIG Wrapper Notes This function is attached as method `eval_covar_structure()` to objects of type `fold_compound`

15.1.2.3 float vrna_eval_structure_simple (const char * string, const char * structure)

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA.

This function allows for energy evaluation of a given sequence/structure pair. In contrast to `vrna_eval_structure()` this function assumes default model details and default energy parameters in order to evaluate the free energy of the secondary structure. Therefore, it serves as a simple interface function for energy evaluation for situations where no changes on the energy model are required.

See also

[vrna_eval_structure\(\)](#), [vrna_eval_structure_pt\(\)](#), [vrna_eval_structure_verbose\(\)](#), [vrna_eval_structure_pt_verbose\(\)](#),

Parameters

<i>string</i>	RNA sequence in uppercase letters
<i>structure</i>	Secondary structure in dot-bracket notation

Returns

The free energy of the input structure given the input sequence in kcal/mol

15.1.2.4 `float vrna_eval_structure_verbose (vrna_fold_compound_t * vc, const char * structure, FILE * file)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA and print contributions on a per-loop base.

This function is a simplified version of [vrna_eval_structure_v\(\)](#) that uses the *default* verbosity level. (

See also

[vrna_eval_structure_pt\(\)](#), [vrna_eval_structure_verbose\(\)](#), [vrna_eval_structure_pt_verbose\(\)](#),

Parameters

<i>vc</i>	A <code>vrna_fold_compound_t</code> containing the energy parameters and model details
<i>structure</i>	Secondary structure in dot-bracket notation
<i>file</i>	A file handle where this function should print to (may be NULL).

Returns

The free energy of the input structure given the input sequence in kcal/mol

SWIG Wrapper Notes This function is attached as method `eval_structure_verbose()` to objects of type `fold_compound`

15.1.2.5 `float vrna_eval_structure_v (vrna_fold_compound_t * vc, const char * structure, int verbosity_level, FILE * file)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA and print contributions on a per-loop base.

This function allows for detailed energy evaluation of a given sequence/structure pair. In contrast to [vrna_eval_structure\(\)](#) this function prints detailed energy contributions based on individual loops to a file handle. If NULL is passed as file handle, this function defaults to print to stdout. Any positive `verbosity_level` activates potential warning message of the energy evaluating functions, while values ≥ 1 allow for detailed control of what data is printed. A negative parameter `verbosity_level` turns off printing all together.

Model details, energy parameters, and possibly soft constraints are used as provided via the parameter 'vc'. The `fold_compound` does not need to contain any DP matrices, but all the most basic init values as one would get from a call like this:

```
vc = vrna_fold_compound(sequence, NULL, VRNA_OPTION_EVAL_ONLY);
```


See also

[vrna_eval_structure_pt\(\)](#), [vrna_eval_structure_verbose\(\)](#), [vrna_eval_structure_pt_verbose\(\)](#),

Parameters

<i>vc</i>	A <code>vrna_fold_compound_t</code> containing the energy parameters and model details
<i>structure</i>	Secondary structure in dot-bracket notation
<i>verbosity_level</i>	The level of verbosity of this function
<i>file</i>	A file handle where this function should print to (may be NULL).

Returns

The free energy of the input structure given the input sequence in kcal/mol

15.1.2.6 `float vrna_eval_structure_simple_verbose (const char * string, const char * structure, FILE * file)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA and print contributions per loop.

This function is a simplified version of [vrna_eval_structure_simple_v\(\)](#) that uses the *default* verbosity level.

See also

[vrna_eval_structure_simple_v\(\)](#), [vrna_eval_structure_verbose\(\)](#), [vrna_eval_structure_pt\(\)](#), [vrna_eval_structure_pt_verbose\(\)](#), [vrna_eval_structure_verbose\(\)](#), [vrna_eval_structure_pt_verbose\(\)](#)

Parameters

<i>string</i>	RNA sequence in uppercase letters
<i>structure</i>	Secondary structure in dot-bracket notation
<i>file</i>	A file handle where this function should print to (may be NULL).

Returns

The free energy of the input structure given the input sequence in kcal/mol

15.1.2.7 `float vrna_eval_structure_simple_v (const char * string, const char * structure, int verbosity_level, FILE * file)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA and print contributions per loop.

This function allows for detailed energy evaluation of a given sequence/structure pair. In contrast to [vrna_eval_structure\(\)](#) this function prints detailed energy contributions based on individual loops to a file handle. If NULL is passed as file handle, this function defaults to print to stdout. Any positive `verbosity_level` activates potential warning message of the energy evaluating functions, while values ≥ 1 allow for detailed control of what data is printed. A negative parameter `verbosity_level` turns off printing all together.

In contrast to [vrna_eval_structure_verbose\(\)](#) this function assumes default model details and default energy parameters in order to evaluate the free energy of the secondary structure. Therefore, it serves as a simple interface function for energy evaluation for situations where no changes on the energy model are required.

See also

[vrna_eval_structure_verbose\(\)](#), [vrna_eval_structure_pt\(\)](#), [vrna_eval_structure_verbose\(\)](#), [vrna_eval_structure_pt_verbose\(\)](#),

Parameters

<i>string</i>	RNA sequence in uppercase letters
<i>structure</i>	Secondary structure in dot-bracket notation
<i>verbosity_level</i>	The level of verbosity of this function
<i>file</i>	A file handle where this function should print to (may be NULL).

Returns

The free energy of the input structure given the input sequence in kcal/mol

15.1.2.8 `int vrna_eval_structure_pt (vrna_fold_compound_t * vc, const short * pt)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA.

This function allows for energy evaluation of a given sequence/structure pair where the structure is provided in pair_table format as obtained from [vrna_ptable\(\)](#). Model details, energy parameters, and possibly soft constraints are used as provided via the parameter 'vc'. The fold_compound does not need to contain any DP matrices, but all the most basic init values as one would get from a call like this:

```
vc = vrna_fold_compound(sequence, NULL, VRNA_OPTION_EVAL_ONLY);
```

See also

[vrna_ptable\(\)](#), [vrna_eval_structure\(\)](#), [vrna_eval_structure_pt_verbose\(\)](#)

Parameters

<i>vc</i>	A vrna_fold_compound_t containing the energy parameters and model details
<i>pt</i>	Secondary structure as pair_table

Returns

The free energy of the input structure given the input sequence in 10cal/mol

SWIG Wrapper Notes This function is attached as method `eval_structure_pt()` to objects of type *fold_compound*

15.1.2.9 `int vrna_eval_structure_pt_simple (const char * string, const short * pt)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA.

In contrast to [vrna_eval_structure_pt\(\)](#) this function assumes default model details and default energy parameters in order to evaluate the free energy of the secondary structure. Therefore, it serves as a simple interface function for energy evaluation for situations where no changes on the energy model are required.

See also

[vrna_ptable\(\)](#), [vrna_eval_structure_simple\(\)](#), [vrna_eval_structure_pt\(\)](#)

Parameters

<i>string</i>	RNA sequence in uppercase letters
<i>pt</i>	Secondary structure as pair_table

Returns

The free energy of the input structure given the input sequence in 10cal/mol

15.1.2.10 `int vrna_eval_structure_pt_verbose (vrna_fold_compound_t * vc, const short * pt, FILE * file)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA.

This function is a simplified version of [vrna_eval_structure_simple_v\(\)](#) that uses the *default* verbosity level.

See also

[vrna_eval_structure_pt_v\(\)](#), [vrna_ptable\(\)](#), [vrna_eval_structure_pt\(\)](#), [vrna_eval_structure_verbose\(\)](#)

Parameters

<i>vc</i>	A <code>vrna_fold_compound_t</code> containing the energy parameters and model details
<i>pt</i>	Secondary structure as pair_table
<i>file</i>	A file handle where this function should print to (may be NULL).

Returns

The free energy of the input structure given the input sequence in 10cal/mol

SWIG Wrapper Notes This function is attached as method `eval_structure_pt_verbose()` to objects of type `fold↔_compound`

15.1.2.11 `int vrna_eval_structure_pt_v (vrna_fold_compound_t * vc, const short * pt, int verbosity_level, FILE * file)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA.

This function allows for energy evaluation of a given sequence/structure pair where the structure is provided in pair_table format as obtained from [vrna_ptable\(\)](#). Model details, energy parameters, and possibly soft constraints are used as provided via the parameter 'vc'. The fold_compound does not need to contain any DP matrices, but all the most basic init values as one would get from a call like this:

```
vc = vrna_fold_compound(sequence, NULL, VRNA_OPTION_EVAL_ONLY);
```

In contrast to [vrna_eval_structure_pt\(\)](#) this function prints detailed energy contributions based on individual loops to a file handle. If NULL is passed as file handle, this function defaults to print to stdout. Any positive `verbosity_level` activates potential warning message of the energy evaluating functions, while values ≥ 1 allow for detailed control of what data is printed. A negative parameter `verbosity_level` turns off printing all together.

See also

[vrna_ptable\(\)](#), [vrna_eval_structure_pt\(\)](#), [vrna_eval_structure_verbose\(\)](#)

Parameters

<i>vc</i>	A <code>vrna_fold_compound_t</code> containing the energy parameters and model details
<i>pt</i>	Secondary structure as pair_table
<i>verbosity_level</i>	The level of verbosity of this function
<i>file</i>	A file handle where this function should print to (may be NULL).

Returns

The free energy of the input structure given the input sequence in 10cal/mol

15.1.2.12 `int vrna_eval_structure_pt_simple_verbose (const char * string, const short * pt, FILE * file)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA.

This function is a simplified version of [vrna_eval_structure_pt_simple_v\(\)](#) that uses the *default* verbosity level.

See also

[vrna_eval_structure_pt_simple_v\(\)](#), [vrna_ptable\(\)](#), [vrna_eval_structure_pt_verbose\(\)](#), [vrna_eval_structure_pt_simple\(\)](#)

Parameters

<i>string</i>	RNA sequence in uppercase letters
<i>pt</i>	Secondary structure as pair_table
<i>file</i>	A file handle where this function should print to (may be NULL).

Returns

The free energy of the input structure given the input sequence in 10cal/mol

15.1.2.13 `int vrna_eval_structure_pt_simple_v (const char * string, const short * pt, int verbosity_level, FILE * file)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA.

This function allows for energy evaluation of a given sequence/structure pair where the structure is provided in pair_table format as obtained from [vrna_ptable\(\)](#). Model details, energy parameters, and possibly soft constraints are used as provided via the parameter 'vc'. The fold_compound does not need to contain any DP matrices, but all the most basic init values as one would get from a call like this:

```
vc = vrna_fold_compound(sequence, NULL, VRNA_OPTION_EVAL_ONLY);
```

In contrast to [vrna_eval_structure_pt_verbose\(\)](#) this function assumes default model details and default energy parameters in order to evaluate the free energy of the secondary structure. Therefore, it serves as a simple interface function for energy evaluation for situations where no changes on the energy model are required.

See also

[vrna_ptable\(\)](#), [vrna_eval_structure_pt_v\(\)](#), [vrna_eval_structure_simple\(\)](#)

Parameters

<i>string</i>	RNA sequence in uppercase letters
<i>pt</i>	Secondary structure as pair_table
<i>verbosity_level</i>	The level of verbosity of this function
<i>file</i>	A file handle where this function should print to (may be NULL).

Returns

The free energy of the input structure given the input sequence in 10cal/mol

15.1.2.14 `int vrna_eval_loop_pt (vrna_fold_compound_t * vc, int i, const short * pt)`

```
#include <ViennaRNA/eval.h>
```

Calculate energy of a loop.

Parameters

<i>vc</i>	A vrna_fold_compound_t containing the energy parameters and model details
<i>i</i>	position of covering base pair
<i>pt</i>	the pair table of the secondary structure

Returns

free energy of the loop in 10cal/mol

SWIG Wrapper Notes This function is attached as method **eval_loop_pt()** to objects of type *fold_compound*

15.1.2.15 float vrna_eval_move (vrna_fold_compound_t * vc, const char * structure, int m1, int m2)

```
#include <ViennaRNA/eval.h>
```

Calculate energy of a move (closing or opening of a base pair)

If the parameters m1 and m2 are negative, it is deletion (opening) of a base pair, otherwise it is insertion (opening).

See also

[vrna_eval_move_pt\(\)](#)

Parameters

<i>vc</i>	A vrna_fold_compound_t containing the energy parameters and model details
<i>structure</i>	secondary structure in dot-bracket notation
<i>m1</i>	first coordinate of base pair
<i>m2</i>	second coordinate of base pair

Returns

energy change of the move in kcal/mol

SWIG Wrapper Notes This function is attached as method **eval_move()** to objects of type *fold_compound*

15.1.2.16 int vrna_eval_move_pt (vrna_fold_compound_t * vc, short * pt, int m1, int m2)

```
#include <ViennaRNA/eval.h>
```

Calculate energy of a move (closing or opening of a base pair)

If the parameters m1 and m2 are negative, it is deletion (opening) of a base pair, otherwise it is insertion (opening).

See also

[vrna_eval_move\(\)](#)

Parameters

<i>vc</i>	A vrna_fold_compound_t containing the energy parameters and model details
<i>pt</i>	the pair table of the secondary structure
<i>m1</i>	first coordinate of base pair
<i>m2</i>	second coordinate of base pair

Returns

energy change of the move in 10cal/mol

SWIG Wrapper Notes This function is attached as method `eval_move_pt()` to objects of type `fold_compound`

15.1.2.17 float `energy_of_structure` (const char * *string*, const char * *structure*, int *verbosity_level*)

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA using global model detail settings.

If verbosity level is set to a value >0, energies of structure elements are printed to stdout

Note

OpenMP: This function relies on several global model settings variables and thus is not to be considered threadsafe. See `energy_of_struct_par()` for a completely threadsafe implementation.

Deprecated Use `vrna_eval_structure()` or `vrna_eval_structure_verbose()` instead!

See also

[vrna_eval_structure\(\)](#)

Parameters

<i>string</i>	RNA sequence
<i>structure</i>	secondary structure in dot-bracket notation
<i>verbosity_level</i>	a flag to turn verbose output on/off

Returns

the free energy of the input structure given the input sequence in kcal/mol

15.1.2.18 float `energy_of_struct_par` (const char * *string*, const char * *structure*, `vrna_param_t` * *parameters*, int *verbosity_level*)

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA.

If verbosity level is set to a value >0, energies of structure elements are printed to stdout

Deprecated Use `vrna_eval_structure()` or `vrna_eval_structure_verbose()` instead!

See also

[vrna_eval_structure\(\)](#)

Parameters

<i>string</i>	RNA sequence in uppercase letters
<i>structure</i>	Secondary structure in dot-bracket notation
<i>parameters</i>	A data structure containing the prescaled energy contributions and the model details.
<i>verbosity_level</i>	A flag to turn verbose output on/off

Returns

The free energy of the input structure given the input sequence in kcal/mol

15.1.2.19 float `energy_of_circ_structure` (const char * *string*, const char * *structure*, int *verbosity_level*)

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded circular RNA.

Note

OpenMP: This function relies on several global model settings variables and thus is not to be considered threadsafe. See [energy_of_circ_struct_par\(\)](#) for a completely threadsafe implementation.

If verbosity level is set to a value >0, energies of structure elements are printed to stdout

Deprecated Use [vrna_eval_structure\(\)](#) or [vrna_eval_structure_verbose\(\)](#) instead!

See also

[vrna_eval_structure\(\)](#)

Parameters

<i>string</i>	RNA sequence
<i>structure</i>	Secondary structure in dot-bracket notation
<i>verbosity_level</i>	A flag to turn verbose output on/off

Returns

The free energy of the input structure given the input sequence in kcal/mol

15.1.2.20 float `energy_of_circ_struct_par` (const char * *string*, const char * *structure*, `vrna_param_t` * *parameters*, int *verbosity_level*)

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded circular RNA.

If verbosity level is set to a value >0, energies of structure elements are printed to stdout

Deprecated Use [vrna_eval_structure\(\)](#) or [vrna_eval_structure_verbose\(\)](#) instead!

See also

[vrna_eval_structure\(\)](#)

Parameters

<i>string</i>	RNA sequence
<i>structure</i>	Secondary structure in dot-bracket notation
<i>parameters</i>	A data structure containing the prescaled energy contributions and the model details.
<i>verbosity_level</i>	A flag to turn verbose output on/off

Returns

The free energy of the input structure given the input sequence in kcal/mol

15.1.2.21 `int energy_of_structure_pt (const char * string, short * ptable, short * s, short * s1, int verbosity_level)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA.

If verbosity level is set to a value >0, energies of structure elements are printed to stdout

Note

OpenMP: This function relies on several global model settings variables and thus is not to be considered threadsafe. See [energy_of_struct_pt_par\(\)](#) for a completely threadsafe implementation.

Deprecated Use [vrna_eval_structure_pt\(\)](#) or [vrna_eval_structure_pt_verbose\(\)](#) instead!

See also

[vrna_eval_structure_pt\(\)](#)

Parameters

<i>string</i>	RNA sequence
<i>ptable</i>	the pair table of the secondary structure
<i>s</i>	encoded RNA sequence
<i>s1</i>	encoded RNA sequence
<i>verbosity_level</i>	a flag to turn verbose output on/off

Returns

the free energy of the input structure given the input sequence in 10kcal/mol

15.1.2.22 `int energy_of_struct_pt_par (const char * string, short * ptable, short * s, short * s1, vrna_param_t * parameters, int verbosity_level)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA.

If verbosity level is set to a value >0, energies of structure elements are printed to stdout

Deprecated Use `vrna_eval_structure_pt()` or `vrna_eval_structure_pt_verbose()` instead!

See also

[vrna_eval_structure_pt\(\)](#)

Parameters

<i>string</i>	RNA sequence in uppercase letters
<i>ptable</i>	The pair table of the secondary structure
<i>s</i>	Encoded RNA sequence
<i>s1</i>	Encoded RNA sequence
<i>parameters</i>	A data structure containing the prescaled energy contributions and the model details.
<i>verbosity_level</i>	A flag to turn verbose output on/off

Returns

The free energy of the input structure given the input sequence in 10kcal/mol

15.1.2.23 `float energy_of_move (const char * string, const char * structure, int m1, int m2)`

```
#include <ViennaRNA/eval.h>
```

Calculate energy of a move (closing or opening of a base pair)

If the parameters *m1* and *m2* are negative, it is deletion (opening) of a base pair, otherwise it is insertion (opening).

Deprecated Use `vrna_eval_move()` instead!

See also

[vrna_eval_move\(\)](#)

Parameters

<i>string</i>	RNA sequence
<i>structure</i>	secondary structure in dot-bracket notation
<i>m1</i>	first coordinate of base pair
<i>m2</i>	second coordinate of base pair

Returns

energy change of the move in kcal/mol

15.1.2.24 `int energy_of_move_pt(short * pt, short * s, short * s1, int m1, int m2)`

```
#include <ViennaRNA/eval.h>
```

Calculate energy of a move (closing or opening of a base pair)

If the parameters *m1* and *m2* are negative, it is deletion (opening) of a base pair, otherwise it is insertion (opening).

Deprecated Use `vrna_eval_move_pt()` instead!

See also

[vrna_eval_move_pt\(\)](#)

Parameters

<i>pt</i>	the pair table of the secondary structure
<i>s</i>	encoded RNA sequence
<i>s1</i>	encoded RNA sequence
<i>m1</i>	first coordinate of base pair
<i>m2</i>	second coordinate of base pair

Returns

energy change of the move in 10cal/mol

15.1.2.25 `int loop_energy(short * ptable, short * s, short * s1, int i)`

```
#include <ViennaRNA/eval.h>
```

Calculate energy of a loop.

Deprecated Use `vrna_eval_loop_pt()` instead!

See also

[vrna_eval_loop_pt\(\)](#)

Parameters

<i>ptable</i>	the pair table of the secondary structure
<i>s</i>	encoded RNA sequence
<i>s1</i>	encoded RNA sequence
<i>i</i>	position of covering base pair

Returns

free energy of the loop in 10cal/mol

15.1.2.26 float `energy_of_struct (const char * string, const char * structure)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA

Note

This function is not entirely threadsafe! Depending on the state of the global variable `eos_debug` it prints energy information to stdout or not...

Deprecated This function is deprecated and should not be used in future programs! Use `energy_of_structure()` instead!

See also

`energy_of_structure`, `energy_of_circ_struct()`, `energy_of_struct_pt()`

Parameters

<i>string</i>	RNA sequence
<i>structure</i>	secondary structure in dot-bracket notation

Returns

the free energy of the input structure given the input sequence in kcal/mol

15.1.2.27 int `energy_of_struct_pt (const char * string, short * ptable, short * s, short * s1)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded RNA

Note

This function is not entirely threadsafe! Depending on the state of the global variable `eos_debug` it prints energy information to stdout or not...

Deprecated This function is deprecated and should not be used in future programs! Use `energy_of_structure_pt()` instead!

See also

`make_pair_table()`, `energy_of_structure()`

Parameters

<i>string</i>	RNA sequence
<i>ptable</i>	the pair table of the secondary structure
<i>s</i>	encoded RNA sequence
<i>s1</i>	encoded RNA sequence

Returns

the free energy of the input structure given the input sequence in 10kcal/mol

15.1.2.28 `float energy_of_circ_struct (const char * string, const char * structure)`

```
#include <ViennaRNA/eval.h>
```

Calculate the free energy of an already folded circular RNA

Note

This function is not entirely threadsafe! Depending on the state of the global variable `eos_debug` it prints energy information to stdout or not...

Deprecated This function is deprecated and should not be used in future programs Use `energy_of_circ_structure()` instead!

See also

`energy_of_circ_structure()`, `energy_of_struct()`, `energy_of_struct_pt()`

Parameters

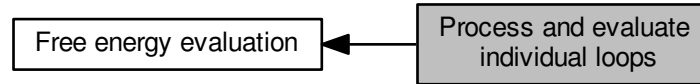
<i>string</i>	RNA sequence
<i>structure</i>	secondary structure in dot-bracket notation

Returns

the free energy of the input structure given the input sequence in kcal/mol

15.2 Process and evaluate individual loops

Collaboration diagram for Process and evaluate individual loops:



Files

- file [exterior_loops.h](#)
Energy evaluation of exterior loops for MFE and partition function calculations.
- file [hairpin_loops.h](#)
Energy evaluation of hairpin loops for MFE and partition function calculations.
- file [interior_loops.h](#)
Energy evaluation of interior loops for MFE and partition function calculations.
- file [loop_energies.h](#)
Energy evaluation for MFE and partition function calculations.
- file [multibranch_loops.h](#)
Energy evaluation of multibranch loops for MFE and partition function calculations.

- `int E_ExtLoop (int type, int si1, int sj1, vrna_param_t *P)`
- `FLT_OR_DBL exp_E_ExtLoop (int type, int si1, int sj1, vrna_exp_param_t *P)`
- `int E_Stem (int type, int si1, int sj1, int extLoop, vrna_param_t *P)`
- `FLT_OR_DBL exp_E_Stem (int type, int si1, int sj1, int extLoop, vrna_exp_param_t *P)`

- `PRIVATE int E_Hairpin (int size, int type, int si1, int sj1, const char *string, vrna_param_t *P)`
Compute the Energy of a hairpin-loop.
- `int vrna_eval_ext_hp_loop (vrna_fold_compound_t *vc, int i, int j)`
Evaluate free energy of an exterior hairpin loop.
- `int vrna_eval_hp_loop (vrna_fold_compound_t *vc, int i, int j)`
Evaluate free energy of a hairpin loop.
- `PRIVATE FLT_OR_DBL exp_E_Hairpin (int u, int type, short si1, short sj1, const char *string, vrna_exp_param_t *P)`
Compute Boltzmann weight $e^{-\Delta G/kT}$ of a hairpin loop.
- `int vrna_E_hp_loop (vrna_fold_compound_t *vc, int i, int j)`
Evaluate the free energy of a hairpin loop and consider hard constraints if they apply.
- `int vrna_E_ext_hp_loop (vrna_fold_compound_t *vc, int i, int j)`
Evaluate the free energy of an exterior hairpin loop and consider possible hard constraints.
- `FLT_OR_DBL vrna_exp_E_hp_loop (vrna_fold_compound_t *vc, int i, int j)`
High-Level function for hairpin loop energy evaluation (partition function variant)
- `int vrna_BT_hp_loop (vrna_fold_compound_t *vc, int i, int j, int en, vrna_bp_stack_t *bp_stack, int *stack_count)`

Backtrack a hairpin loop closed by (i, j) .

- PRIVATE int [E_IntLoop](#) (int n1, int n2, int type, int type_2, int si1, int sj1, int sp1, int sq1, [vrna_param_t](#) *P)
- PRIVATE FLT_OR_DBL [exp_E_IntLoop](#) (int u1, int u2, int type, int type2, short si1, short sj1, short sp1, short sq1, [vrna_exp_param_t](#) *P)
- int [vrna_eval_int_loop](#) ([vrna_fold_compound_t](#) *vc, int i, int j, int k, int l)
- int [vrna_BT_stack](#) ([vrna_fold_compound_t](#) *vc, int *i, int *j, int *en, [vrna_bp_stack_t](#) *bp_stack, int *stack_count)

Backtrack a stacked pair closed by (i, j) .

- int [vrna_BT_int_loop](#) ([vrna_fold_compound_t](#) *vc, int *i, int *j, int en, [vrna_bp_stack_t](#) *bp_stack, int *stack_count)

Backtrack an interior loop closed by (i, j) .

15.2.1 Detailed Description

15.2.2 Function Documentation

15.2.2.1 int [E_ExtLoop](#) (int type, int si1, int sj1, [vrna_param_t](#) * P)

```
#include <ViennaRNA/exterior\_loops.h>
```

Compute the Energy contribution of an Exterior loop stem

This definition is a wrapper for the [E_Stem\(\)](#) function. It is substituted by an [E_Stem\(\)](#) function call with argument extLoop=1, so the energy contribution returned reflects a stem introduced in an exterior-loop.

As for the parameters si1 and sj1 of the substituted [E_Stem\(\)](#) function, you can inhibit to take 5'-, 3'-dangles or mismatch contributions to be taken into account by passing -1 to these parameters.

See also

[E_Stem\(\)](#)

Parameters

<i>type</i>	The pair type of the stem-closing pair
<i>si1</i>	The 5'-mismatching nucleotide
<i>sj1</i>	The 3'-mismatching nucleotide
<i>P</i>	The data structure containing scaled energy parameters

Returns

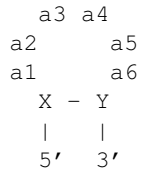
The energy contribution of the introduced exterior-loop stem

15.2.2.2 PRIVATE int [E_Hairpin](#) (int size, int type, int si1, int sj1, const char * string, [vrna_param_t](#) * P)

```
#include <ViennaRNA/hairpin\_loops.h>
```


Compute the Energy of a hairpin-loop.

To evaluate the free energy of a hairpin-loop, several parameters have to be known. A general hairpin-loop has this structure:



where X-Y marks the closing pair [e.g. a (**G,C**) pair]. The length of this loop is 6 as there are six unpaired nucleotides (a1-a6) enclosed by (X,Y). The 5' mismatching nucleotide is a1 while the 3' mismatch is a6. The nucleotide sequence of this loop is "a1.a2.a3.a4.a5.a6"

Note

The parameter sequence should contain the sequence of the loop in capital letters of the nucleic acid alphabet if the loop size is below 7. This is useful for unusually stable tri-, tetra- and hexa-loops which are treated differently (based on experimental data) if they are tabulated.

See also

[scale_parameters\(\)](#)
[vrna_param_t](#)

Warning

Not (really) thread safe! A threadsafe implementation will replace this function in a future release!
 Energy evaluation may change due to updates in global variable "tetra_loop"

Parameters

<i>size</i>	The size of the loop (number of unpaired nucleotides)
<i>type</i>	The pair type of the base pair closing the hairpin
<i>si1</i>	The 5'-mismatching nucleotide
<i>sj1</i>	The 3'-mismatching nucleotide
<i>string</i>	The sequence of the loop
<i>P</i>	The datastructure containing scaled energy parameters

Returns

The Free energy of the Hairpin-loop in dcal/mol

15.2.2.3 `int vrna_eval_hp_loop (vrna_fold_compound_t * vc, int i, int j)`

```
#include <ViennaRNA/hairpin_loops.h>
```

Evaluate free energy of a hairpin loop.

Note

This function is polymorphic! The provided `vrna_fold_compound_t` may be of type `VRNA_FC_TYPE_SINGLE` or `VRNA_FC_TYPE_COMPARATIVE`

Parameters

<i>vc</i>	The <code>vrna_fold_compound_t</code> for the particular energy evaluation
<i>i</i>	5'-position of the base pair
<i>j</i>	3'-position of the base pair

Returns

Free energy of the hairpin loop closed by (i, j) in deka-kal/mol

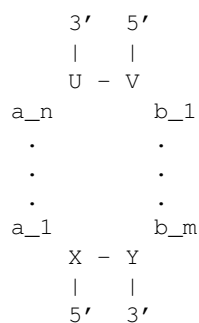
SWIG Wrapper Notes This function is attached as method `eval_hp_loop()` to objects of type `fold_compound`

15.2.2.4 PRIVATE int E_IntLoop (int *n1*, int *n2*, int *type*, int *type_2*, int *si1*, int *sj1*, int *sp1*, int *sq1*, vrna_param_t * *P*)

```
#include <ViennaRNA/interior_loops.h>
```

Compute the Energy of an interior-loop

This function computes the free energy ΔG of an interior-loop with the following structure:



This general structure depicts an interior-loop that is closed by the base pair (X,Y). The enclosed base pair is (V,U) which leaves the unpaired bases a_1 - a_n and b_1 - b_n that constitute the loop. In this example, the length of the interior-loop is $(n + m)$ where n or m may be 0 resulting in a bulge-loop or base pair stack. The mismatching nucleotides for the closing pair (X,Y) are:

5'-mismatch: a_1

3'-mismatch: b_m

and for the enclosed base pair (V,U):

5'-mismatch: b_1

3'-mismatch: a_n

Note

Base pairs are always denoted in 5'->3' direction. Thus the enclosed base pair must be 'turned around' when evaluating the free energy of the interior-loop

See also

[scale_parameters\(\)](#)
[vrna_param_t](#)

Note

This function is threadsafe

Parameters

<i>n1</i>	The size of the 'left'-loop (number of unpaired nucleotides)
<i>n2</i>	The size of the 'right'-loop (number of unpaired nucleotides)
<i>type</i>	The pair type of the base pair closing the interior loop
<i>type</i> _↔ <i>_2</i>	The pair type of the enclosed base pair
<i>si1</i>	The 5'-mismatching nucleotide of the closing pair
<i>sj1</i>	The 3'-mismatching nucleotide of the closing pair
<i>sp1</i>	The 3'-mismatching nucleotide of the enclosed pair
<i>sq1</i>	The 5'-mismatching nucleotide of the enclosed pair
<i>P</i>	The datastructure containing scaled energy parameters

Returns

The Free energy of the Interior-loop in dcal/mol

15.2.2.5 FLT_OR_DBL exp_E_ExtLoop (int *type*, int *si1*, int *sj1*, vrna_exp_param_t * *P*)

```
#include <ViennaRNA/exterior_loops.h>
```

This is the partition function variant of [E_ExtLoop\(\)](#)

See also

[E_ExtLoop\(\)](#)

Returns

The Boltzmann weighted energy contribution of the introduced exterior-loop stem

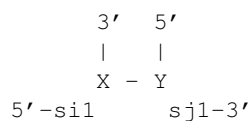
15.2.2.6 int E_Stem (int *type*, int *si1*, int *sj1*, int *extLoop*, vrna_param_t * *P*)

```
#include <ViennaRNA/exterior_loops.h>
```

Compute the energy contribution of a stem branching off a loop-region

This function computes the energy contribution of a stem that branches off a loop region. This can be the case in multiloops, when a stem branching off increases the degree of the loop but also *immediately interior base pairs* of an exterior loop contribute free energy. To switch the behavior of the function according to the evaluation of a multiloop- or exterior-loop-stem, you pass the flag 'extLoop'. The returned energy contribution consists of a TerminalAU penalty if the pair type is greater than 2, dangling end contributions of mismatching nucleotides adjacent to the stem if only one of the si1, sj1 parameters is greater than 0 and mismatch energies if both mismatching nucleotides are positive values. Thus, to avoid incorporating dangling end or mismatch energies just pass a negative number, e.g. -1 to the mismatch argument.

This is an illustration of how the energy contribution is assembled:



Here, (X,Y) is the base pair that closes the stem that branches off a loop region. The nucleotides si1 and sj1 are the 5'- and 3'- mismatches, respectively. If the base pair type of (X,Y) is greater than 2 (i.e. an A-U or G-U pair, the TerminalAU penalty will be included in the energy contribution returned. If si1 and sj1 are both nonnegative numbers, mismatch energies will also be included. If one of si1 or sj1 is a negative value, only 5' or 3' dangling end contributions are taken into account. To prohibit any of these mismatch contributions to be incorporated, just pass a negative number to both, si1 and sj1. In case the argument extLoop is 0, the returned energy contribution also includes the *internal-loop-penalty* of a multiloop stem with closing pair type.

See also

[E_MLstem\(\)](#)
[E_ExtLoop\(\)](#)

Note

This function is threadsafe

Parameters

<i>type</i>	The pair type of the first base pair on the stem
<i>si1</i>	The 5'-mismatching nucleotide
<i>sj1</i>	The 3'-mismatching nucleotide
<i>extLoop</i>	A flag that indicates whether the contribution reflects the one of an exterior loop or not
<i>P</i>	The data structure containing scaled energy parameters

Returns

The Free energy of the branch off the loop in dcal/mol

15.2.2.7 FLT_OR_DBL exp_E_Stem (int type, int si1, int sj1, int extLoop, vrna_exp_param_t * P)

```
#include <ViennaRNA/exterior_loops.h>
```

Compute the Boltzmann weighted energy contribution of a stem branching off a loop-region

This is the partition function variant of [E_Stem\(\)](#)

See also

[E_Stem\(\)](#)

Note

This function is threadsafe

Returns

The Boltzmann weighted energy contribution of the branch off the loop

**15.2.2.8 PRIVATE FLT_OR_DBL exp_E_Hairpin (int *u*, int *type*, short *si1*, short *sj1*, const char * *string*,
vrna_exp_param_t * *P*)**

```
#include <ViennaRNA/hairpin_loops.h>
```

Compute Boltzmann weight $e^{-\Delta G/kT}$ of a hairpin loop.

multiply by scale[u+2]

See also

[get_scaled_pf_parameters\(\)](#)
[vrna_exp_param_t](#)
[E_Hairpin\(\)](#)

Warning

Not (really) thread safe! A threadsafe implementation will replace this function in a future release!
Energy evaluation may change due to updates in global variable "tetra_loop"

Parameters

<i>u</i>	The size of the loop (number of unpaired nucleotides)
<i>type</i>	The pair type of the base pair closing the hairpin
<i>si1</i>	The 5'-mismatching nucleotide
<i>sj1</i>	The 3'-mismatching nucleotide
<i>string</i>	The sequence of the loop
<i>P</i>	The datastructure containing scaled Boltzmann weights of the energy parameters

Returns

The Boltzmann weight of the Hairpin-loop

15.2.2.9 `int vrna_E_hp_loop (vrna_fold_compound_t * vc, int i, int j)`

```
#include <ViennaRNA/hairpin_loops.h>
```

Evaluate the free energy of a hairpin loop and consider hard constraints if they apply.

This function evaluates the free energy of a hairpin loop

In case the base pair is not allowed due to a constraint conflict, this function returns `INF`.

Note

This function is polymorphic! The provided `vrna_fold_compound_t` may be of type `VRNA_FC_TYPE_SINGLE` or `VRNA_FC_TYPE_COMPARATIVE`

Parameters

<code>vc</code>	The <code>vrna_fold_compound_t</code> that stores all relevant model settings
<code>i</code>	The 5' nucleotide of the base pair (3' to evaluate the pair as exterior hairpin loop)
<code>j</code>	The 3' nucleotide of the base pair (5' to evaluate the pair as exterior hairpin loop)

Returns

The free energy of the hairpin loop in 10cal/mol

15.2.2.10 `int vrna_E_ext_hp_loop (vrna_fold_compound_t * vc, int i, int j)`

```
#include <ViennaRNA/hairpin_loops.h>
```

Evaluate the free energy of an exterior hairpin loop and consider possible hard constraints.

Note

This function is polymorphic! The provided `vrna_fold_compound_t` may be of type `VRNA_FC_TYPE_SINGLE` or `VRNA_FC_TYPE_COMPARATIVE`

15.2.2.11 `FLT_OR_DBL vrna_exp_E_hp_loop (vrna_fold_compound_t * vc, int i, int j)`

```
#include <ViennaRNA/hairpin_loops.h>
```

High-Level function for hairpin loop energy evaluation (partition function variant)

See also

`vrna_E_hp_loop()` for it's free energy counterpart

Note

This function is polymorphic! The provided `vrna_fold_compound_t` may be of type `VRNA_FC_TYPE_SINGLE` or `VRNA_FC_TYPE_COMPARATIVE`

15.2.2.12 `int vrna_BT_hp_loop (vrna_fold_compound_t * vc, int i, int j, int en, vrna_bp_stack_t * bp_stack, int * stack_count)`

```
#include <ViennaRNA/hairpin_loops.h>
```

Backtrack a hairpin loop closed by (i, j) .

Note

This function is polymorphic! The provided `vrna_fold_compound_t` may be of type `VRNA_FC_TYPE_SINGLE` or `VRNA_FC_TYPE_COMPARATIVE`

15.2.2.13 `PRIVATE FLT_OR_DBL exp_E_IntLoop (int u1, int u2, int type, int type2, short si1, short sj1, short sp1, short sq1, vrna_exp_param_t * P)`

```
#include <ViennaRNA/interior_loops.h>
```

Compute Boltzmann weight $e^{-\Delta G/kT}$ of interior loop

multiply by `scale[u1+u2+2]` for scaling

See also

```
get_scaled_pf_parameters()
vrna_exp_param_t
E_IntLoop()
```

Note

This function is threadsafe

Parameters

<i>u1</i>	The size of the 'left'-loop (number of unpaired nucleotides)
<i>u2</i>	The size of the 'right'-loop (number of unpaired nucleotides)
<i>type</i>	The pair type of the base pair closing the interior loop
<i>type2</i>	The pair type of the enclosed base pair
<i>si1</i>	The 5'-mismatching nucleotide of the closing pair
<i>sj1</i>	The 3'-mismatching nucleotide of the closing pair
<i>sp1</i>	The 3'-mismatching nucleotide of the enclosed pair
<i>sq1</i>	The 5'-mismatching nucleotide of the enclosed pair
<i>P</i>	The datastructure containing scaled Boltzmann weights of the energy parameters

Returns

The Boltzmann weight of the Interior-loop

15.2.2.14 `int vrna_eval_int_loop (vrna_fold_compound_t * vc, int i, int j, int k, int l)`

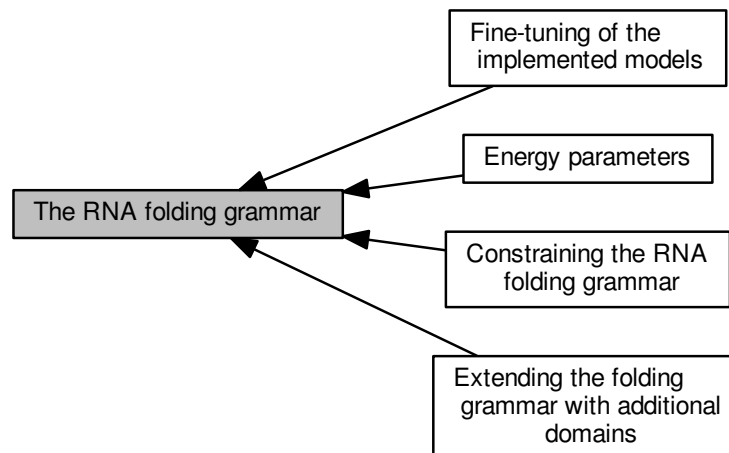
```
#include <ViennaRNA/interior_loops.h>
```

SWIG Wrapper Notes This function is attached as method **eval_int_loop()** to objects of type *fold_compound*

15.3 The RNA folding grammar

The RNA folding grammar as implemented in RNAlib.

Collaboration diagram for The RNA folding grammar:



Modules

- [Fine-tuning of the implemented models](#)

Functions and data structures to fine-tune the implemented secondary structure evaluation model.

- [Energy parameters](#)

All relevant functions to retrieve and copy pre-calculated energy parameter sets as well as reading/writing the energy parameter set from/to file(s).

- [Extending the folding grammar with additional domains](#)

This module covers simple and straight-forward extensions to the RNA folding grammar.

- [Constraining the RNA folding grammar](#)

This module provides general functions that allow for an easy control of constrained secondary structure prediction and evaluation.

Files

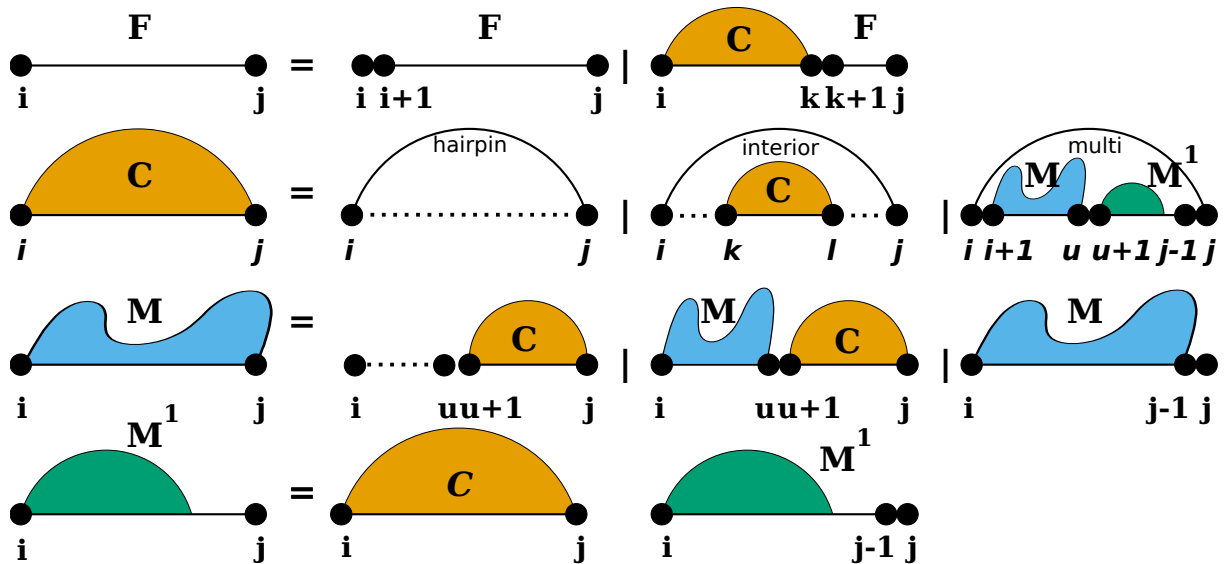
- file [grammar.h](#)

Implementations for the RNA folding grammar.

15.3.1 Detailed Description

The RNA folding grammar as implemented in RNAlib.

This module is split into different aspects of how to modify and manipulate the underlying RNA folding grammar.

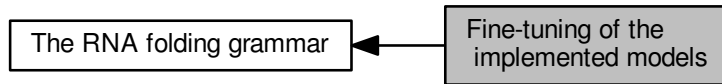


- [Extending the folding grammar with additional domains](#), and
- [Constraining the RNA folding grammar](#)

15.4 Fine-tuning of the implemented models

Functions and data structures to fine-tune the implemented secondary structure evaluation model.

Collaboration diagram for Fine-tuning of the implemented models:



Files

- file `model.h`
The model details data structure and its corresponding modifiers.
- `#define VRNA_MODEL_DEFAULT_TEMPERATURE 37.0`
Default temperature for structure prediction and free energy evaluation in °C
- `#define VRNA_MODEL_DEFAULT_PF_SCALE -1`
Default scaling factor for partition function computations.
- `#define VRNA_MODEL_DEFAULT_BETA_SCALE 1.`
Default scaling factor for absolute thermodynamic temperature in Boltzmann factors.
- `#define VRNA_MODEL_DEFAULT_DANGLES 2`
Default dangling end model.
- `#define VRNA_MODEL_DEFAULT_SPECIAL_HP 1`
Default model behavior for lookup of special tri-, tetra-, and hexa-loops.
- `#define VRNA_MODEL_DEFAULT_NO_LP 0`
Default model behavior for so-called 'lonely pairs'.
- `#define VRNA_MODEL_DEFAULT_NO_GU 0`
Default model behavior for G-U base pairs.
- `#define VRNA_MODEL_DEFAULT_NO_GU_CLOSURE 0`
Default model behavior for G-U base pairs closing a loop.
- `#define VRNA_MODEL_DEFAULT_CIRC 0`
Default model behavior to treat a molecule as a circular RNA (DNA)
- `#define VRNA_MODEL_DEFAULT_GQUAD 0`
Default model behavior regarding the treatment of G-Quadruplexes.
- `#define VRNA_MODEL_DEFAULT_UNIQ_ML 0`
Default behavior of the model regarding unique multi-branch loop decomposition.
- `#define VRNA_MODEL_DEFAULT_ENERGY_SET 0`
Default model behavior on which energy set to use.
- `#define VRNA_MODEL_DEFAULT_BACKTRACK 1`
Default model behavior with regards to backtracking of structures.
- `#define VRNA_MODEL_DEFAULT_BACKTRACK_TYPE 'F'`
Default model behavior on what type of backtracking to perform.
- `#define VRNA_MODEL_DEFAULT_COMPUTE_BPP 1`

- Default model behavior with regards to computing base pair probabilities.*

 - #define `VRNA_MODEL_DEFAULT_MAX_BP_SPAN` -1

Default model behavior for the allowed maximum base pair span.
- #define `VRNA_MODEL_DEFAULT_WINDOW_SIZE` -1

Default model behavior for the sliding window approach.
- #define `VRNA_MODEL_DEFAULT_LOG_ML` 0

Default model behavior on how to evaluate the energy contribution of multi-branch loops.
- #define `VRNA_MODEL_DEFAULT_ALI_OLD_EN` 0

Default model behavior for consensus structure energy evaluation.
- #define `VRNA_MODEL_DEFAULT_ALI_RIBO` 0

Default model behavior for consensus structure co-variance contribution assessment.
- #define `VRNA_MODEL_DEFAULT_ALI_CV_FACT` 1.

Default model behavior for weighting the co-variance score in consensus structure prediction.
- #define `VRNA_MODEL_DEFAULT_ALI_NC_FACT` 1.

Default model behavior for weighting the nucleotide conservation? in consensus structure prediction.
- #define `MAXALPHA` 20

Maximal length of alphabet.
- typedef struct `vrna_md_s vrna_md_t`

Typename for the model details data structure `vrna_md_s`.
- double `temperature`

Rescale energy parameters to a temperature in degC.
- double `pf_scale`

A scaling factor used by `pf_fold()` to avoid overflows.
- int `dangles`

Switch the energy model for dangling end contributions (0, 1, 2, 3)
- int `tetra_loop`

Include special stabilizing energies for some tri-, tetra- and hexa-loops;.
- int `noLonelyPairs`

Global switch to avoid/allow helices of length 1.
- int `noGU`

Global switch to forbid/allow GU base pairs at all.
- int `no_closingGU`

GU allowed only inside stacks if set to 1.
- int `circ`

backward compatibility variable.. this does not effect anything
- int `gquad`

Allow G-quadruplex formation.
- int `canonicalBPonly`
- int `uniq_ML`

do ML decomposition uniquely (for subopt)
- int `energy_set`

0 = BP; 1=any with GC; 2=any with AU-parameter
- int `do_backtrack`

do backtracking, i.e. compute secondary structures or base pair probabilities
- char `backtrack_type`

A backtrack array marker for `inverse_fold()`
- char * `nonstandards`

contains allowed non standard base pairs
- int `max_bp_span`

Maximum allowed base pair span.
- int `oldAliEn`

- use old alifold energies (with gaps)*
- int `ribo`
 - use ribosum matrices*
- int `logML`
 - if nonzero use logarithmic ML energy in energy_of_struct*
- void `vrna_md_set_default` (`vrna_md_t` *md)
 - Apply default model details to a provided vrna_md_t data structure.*
- void `vrna_md_update` (`vrna_md_t` *md)
 - Update the model details data structure.*
- `vrna_md_t` * `vrna_md_copy` (`vrna_md_t` *md_to, const `vrna_md_t` *md_from)
 - Copy/Clone a vrna_md_t model.*
- char * `vrna_md_option_string` (`vrna_md_t` *md)
 - Get a corresponding cmdline parameter string of the options in a vrna_md_t.*
- void `vrna_md_defaults_reset` (`vrna_md_t` *md_p)
 - Reset the global default model details to a specific set of parameters, or their initial values.*
- void `vrna_md_defaults_temperature` (double T)
 - Set default temperature for energy evaluation of loops.*
- double `vrna_md_defaults_temperature_get` (void)
 - Get default temperature for energy evaluation of loops.*
- void `vrna_md_defaults_betaScale` (double b)
 - Set default scaling factor of thermodynamic temperature in Boltzmann factors.*
- double `vrna_md_defaults_betaScale_get` (void)
 - Get default scaling factor of thermodynamic temperature in Boltzmann factors.*
- void `vrna_md_defaults_dangles` (int d)
 - Set default dangle model for structure prediction.*
- int `vrna_md_defaults_dangles_get` (void)
 - Get default dangle model for structure prediction.*
- void `vrna_md_defaults_special_hp` (int flag)
 - Set default behavior for lookup of tabulated free energies for special hairpin loops, such as Tri-, Tetra-, or Hexa-loops.*
- int `vrna_md_defaults_special_hp_get` (void)
 - Get default behavior for lookup of tabulated free energies for special hairpin loops, such as Tri-, Tetra-, or Hexa-loops.*
- void `vrna_md_defaults_noLP` (int flag)
 - Set default behavior for prediction of canonical secondary structures.*
- int `vrna_md_defaults_noLP_get` (void)
 - Get default behavior for prediction of canonical secondary structures.*
- void `vrna_md_defaults_noGU` (int flag)
 - Set default behavior for treatment of G-U wobble pairs.*
- int `vrna_md_defaults_noGU_get` (void)
 - Get default behavior for treatment of G-U wobble pairs.*
- void `vrna_md_defaults_noGUclosure` (int flag)
 - Set default behavior for G-U pairs as closing pair for loops.*
- int `vrna_md_defaults_noGUclosure_get` (void)
 - Get default behavior for G-U pairs as closing pair for loops.*
- void `vrna_md_defaults_logML` (int flag)
 - Set default behavior recomputing free energies of multi-branch loops using a logarithmic model.*
- int `vrna_md_defaults_logML_get` (void)
 - Get default behavior recomputing free energies of multi-branch loops using a logarithmic model.*
- void `vrna_md_defaults_circ` (int flag)
 - Set default behavior whether input sequences are circularized.*
- int `vrna_md_defaults_circ_get` (void)
 - Get default behavior whether input sequences are circularized.*

- void [vrna_md_defaults_gquad](#) (int flag)
Set default behavior for treatment of G-Quadruplexes.
- int [vrna_md_defaults_gquad_get](#) (void)
Get default behavior for treatment of G-Quadruplexes.
- void [vrna_md_defaults_uniq_ML](#) (int flag)
Set default behavior for creating additional matrix for unique multi-branch loop prediction.
- int [vrna_md_defaults_uniq_ML_get](#) (void)
Get default behavior for creating additional matrix for unique multi-branch loop prediction.
- void [vrna_md_defaults_energy_set](#) (int e)
Set default energy set.
- int [vrna_md_defaults_energy_set_get](#) (void)
Get default energy set.
- void [vrna_md_defaults_backtrack](#) (int flag)
Set default behavior for whether to backtrack secondary structures.
- int [vrna_md_defaults_backtrack_get](#) (void)
Get default behavior for whether to backtrack secondary structures.
- void [vrna_md_defaults_backtrack_type](#) (char t)
Set default backtrack type, i.e. which DP matrix is used.
- char [vrna_md_defaults_backtrack_type_get](#) (void)
Get default backtrack type, i.e. which DP matrix is used.
- void [vrna_md_defaults_compute_bpp](#) (int flag)
Set the default behavior for whether to compute base pair probabilities after partition function computation.
- int [vrna_md_defaults_compute_bpp_get](#) (void)
Get the default behavior for whether to compute base pair probabilities after partition function computation.
- void [vrna_md_defaults_max_bp_span](#) (int span)
Set default maximal base pair span.
- int [vrna_md_defaults_max_bp_span_get](#) (void)
Get default maximal base pair span.
- void [vrna_md_defaults_min_loop_size](#) (int size)
Set default minimal loop size.
- int [vrna_md_defaults_min_loop_size_get](#) (void)
Get default minimal loop size.
- void [vrna_md_defaults_window_size](#) (int size)
Set default window size for sliding window structure prediction approaches.
- int [vrna_md_defaults_window_size_get](#) (void)
Get default window size for sliding window structure prediction approaches.
- void [vrna_md_defaults_oldAliEn](#) (int flag)
Set default behavior for whether to use old energy model for comparative structure prediction.
- int [vrna_md_defaults_oldAliEn_get](#) (void)
Get default behavior for whether to use old energy model for comparative structure prediction.
- void [vrna_md_defaults_ribo](#) (int flag)
Set default behavior for whether to use Ribosum Scoring in comparative structure prediction.
- int [vrna_md_defaults_ribo_get](#) (void)
Get default behavior for whether to use Ribosum Scoring in comparative structure prediction.
- void [vrna_md_defaults_cv_fact](#) (double factor)
Set the default co-variance scaling factor used in comparative structure prediction.
- double [vrna_md_defaults_cv_fact_get](#) (void)
Get the default co-variance scaling factor used in comparative structure prediction.
- void [vrna_md_defaults_nc_fact](#) (double factor)
- double [vrna_md_defaults_nc_fact_get](#) (void)
- void [vrna_md_defaults_sfact](#) (double factor)

Set the default scaling factor used to avoid under-/overflows in partition function computation.

- double [vrna_md_defaults_sfact_get](#) (void)

Get the default scaling factor used to avoid under-/overflows in partition function computation.

- void [set_model_details](#) ([vrna_md_t](#) *md)

Set default model details.

15.4.1 Detailed Description

Functions and data structures to fine-tune the implemented secondary structure evaluation model.

15.4.2 Macro Definition Documentation

15.4.2.1 `#define VRNA_MODEL_DEFAULT_TEMPERATURE 37.0`

```
#include <ViennaRNA/model.h>
```

Default temperature for structure prediction and free energy evaluation in °C

See also

[vrna_md_t.temperature](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.2 `#define VRNA_MODEL_DEFAULT_PF_SCALE -1`

```
#include <ViennaRNA/model.h>
```

Default scaling factor for partition function computations.

See also

[vrna_exp_param_t.pf_scale](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.3 `#define VRNA_MODEL_DEFAULT_BETA_SCALE 1.`

```
#include <ViennaRNA/model.h>
```

Default scaling factor for absolute thermodynamic temperature in Boltzmann factors.

See also

[vrna_exp_param_t.alpha](#), [vrna_md_t.betaScale](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.4 `#define VRNA_MODEL_DEFAULT_DANGLES 2`

```
#include <ViennaRNA/model.h>
```

Default dangling end model.

See also

[vrna_md_t.dangles](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.5 `#define VRNA_MODEL_DEFAULT_SPECIAL_HP 1`

```
#include <ViennaRNA/model.h>
```

Default model behavior for lookup of special tri-, tetra-, and hexa-loops.

See also

[vrna_md_t.special_hp](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.6 `#define VRNA_MODEL_DEFAULT_NO_LP 0`

```
#include <ViennaRNA/model.h>
```

Default model behavior for so-called 'lonely pairs'.

See also

[vrna_md_t.noLP](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.7 `#define VRNA_MODEL_DEFAULT_NO_GU 0`

```
#include <ViennaRNA/model.h>
```

Default model behavior for G-U base pairs.

See also

[vrna_md_t.noGU](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.8 `#define VRNA_MODEL_DEFAULT_NO_GU_CLOSURE 0`

```
#include <ViennaRNA/model.h>
```

Default model behavior for G-U base pairs closing a loop.

See also

[vrna_md_t.noGUclosure](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.9 #define VRNA_MODEL_DEFAULT_CIRC 0

```
#include <ViennaRNA/model.h>
```

Default model behavior to treat a molecule as a circular RNA (DNA)

See also

[vrna_md_t.circ](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.10 #define VRNA_MODEL_DEFAULT_GQUAD 0

```
#include <ViennaRNA/model.h>
```

Default model behavior regarding the treatment of G-Quadruplexes.

See also

[vrna_md_t.gquad](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.11 #define VRNA_MODEL_DEFAULT_UNIQ_ML 0

```
#include <ViennaRNA/model.h>
```

Default behavior of the model regarding unique multi-branch loop decomposition.

See also

[vrna_md_t.uniq_ML](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.12 #define VRNA_MODEL_DEFAULT_ENERGY_SET 0

```
#include <ViennaRNA/model.h>
```

Default model behavior on which energy set to use.

See also

[vrna_md_t.energy_set](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.13 #define VRNA_MODEL_DEFAULT_BACKTRACK 1

```
#include <ViennaRNA/model.h>
```

Default model behavior with regards to backtracking of structures.

See also

[vrna_md_t.backtrack](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.14 #define VRNA_MODEL_DEFAULT_BACKTRACK_TYPE 'F'

```
#include <ViennaRNA/model.h>
```

Default model behavior on what type of backtracking to perform.

See also

[vrna_md_t.backtrack_type](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.15 #define VRNA_MODEL_DEFAULT_COMPUTE_BPP 1

```
#include <ViennaRNA/model.h>
```

Default model behavior with regards to computing base pair probabilities.

See also

[vrna_md_t.compute_bpp](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.16 #define VRNA_MODEL_DEFAULT_MAX_BP_SPAN -1

```
#include <ViennaRNA/model.h>
```

Default model behavior for the allowed maximum base pair span.

See also

[vrna_md_t.max_bp_span](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.17 #define VRNA_MODEL_DEFAULT_WINDOW_SIZE -1

```
#include <ViennaRNA/model.h>
```

Default model behavior for the sliding window approach.

See also

[vrna_md_t.window_size](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.18 #define VRNA_MODEL_DEFAULT_LOG_ML 0

```
#include <ViennaRNA/model.h>
```

Default model behavior on how to evaluate the energy contribution of multi-branch loops.

See also

[vrna_md_t.logML](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#)

15.4.2.19 #define VRNA_MODEL_DEFAULT_ALI_OLD_EN 0

```
#include <ViennaRNA/model.h>
```

Default model behavior for consensus structure energy evaluation.

See also

```
vrna_md_t.oldAliEn, vrna_md_defaults_reset(), vrna_md_set_default()
```

15.4.2.20 #define VRNA_MODEL_DEFAULT_ALI_RIBO 0

```
#include <ViennaRNA/model.h>
```

Default model behavior for consensus structure co-variance contribution assessment.

See also

```
vrna_md_t.ribo, vrna_md_defaults_reset(), vrna_md_set_default()
```

15.4.2.21 #define VRNA_MODEL_DEFAULT_ALI_CV_FACT 1.

```
#include <ViennaRNA/model.h>
```

Default model behavior for weighting the co-variance score in consensus structure prediction.

See also

```
vrna_md_t.cv_fact, vrna_md_defaults_reset(), vrna_md_set_default()
```

15.4.2.22 #define VRNA_MODEL_DEFAULT_ALI_NC_FACT 1.

```
#include <ViennaRNA/model.h>
```

Default model behavior for weighting the nucleotide conservation? in consensus structure prediction.

See also

```
vrna_md_t.nc_fact, vrna_md_defaults_reset(), vrna_md_set_default()
```

15.4.3 Function Documentation**15.4.3.1 void vrna_md_set_default (vrna_md_t * md)**

```
#include <ViennaRNA/model.h>
```

Apply default model details to a provided [vrna_md_t](#) data structure.

Use this function to initialize a [vrna_md_t](#) data structure with its default values

Parameters

<i>md</i>	A pointer to the data structure that is about to be initialized
-----------	-----------------------------------------------------------------

15.4.3.2 void vrna_md_update (vrna_md_t * md)

```
#include <ViennaRNA/model.h>
```

Update the model details data structure.

This function should be called after changing the [vrna_md_t.energy_set](#) attribute since it re-initializes base pairing related arrays within the [vrna_md_t](#) data structure. In particular, [vrna_md_t.pair](#), [vrna_md_t.alias](#), and [vrna_md_t.rtype](#) are set to the values that correspond to the specified [vrna_md_t.energy_set](#) option

See also

[vrna_md_t](#), [vrna_md_t.energy_set](#), [vrna_md_t.pair](#), [vrna_md_t.rtype](#), [vrna_md_t.alias](#), [vrna_md_set_default\(\)](#)

15.4.3.3 vrna_md_t* vrna_md_copy (vrna_md_t * md_to, const vrna_md_t * md_from)

```
#include <ViennaRNA/model.h>
```

Copy/Clone a [vrna_md_t](#) model.

Use this function to clone a given model either inplace (target container `md_to` given) or create a copy by cloning the source model and returning it (`md_to == NULL`).

Parameters

<i>md_to</i>	The model to be overwritten (if non-NULL and <code>md_to != md_from</code>)
<i>md_from</i>	The model to copy (if non-NULL)

Returns

A pointer to the copy model (or NULL if `md_from == NULL`)

15.4.3.4 char* vrna_md_option_string (vrna_md_t * md)

```
#include <ViennaRNA/model.h>
```

Get a corresponding cmdline parameter string of the options in a [vrna_md_t](#).

Note

This function is not threadsafe!

15.4.3.5 `void vrna_md_defaults_reset (vrna_md_t * md_p)`

```
#include <ViennaRNA/model.h>
```

Reset the global default model details to a specific set of parameters, or their initial values.

This function resets the global default model details to their initial values, i.e. as specified by the ViennaRNA Package release, upon passing NULL as argument. Alternatively it resets them according to a set of provided parameters.

Note

The global default parameters affect all function calls of RNAlib where model details are not explicitly provided. Hence, any change of them is not considered threadsafe

Warning

This function first resets the global default settings to factory defaults, and only then applies user provided settings (if any). User settings that do not meet specifications are skipped.

See also

[vrna_md_set_default\(\)](#), [vrna_md_t](#)

Parameters

<code>md_p</code>	A set of model details to use as global default (if NULL is passed, factory defaults are restored)
-------------------	----------------------------------------------------------------------------------------------------

15.4.3.6 `void vrna_md_defaults_temperature (double T)`

```
#include <ViennaRNA/model.h>
```

Set default temperature for energy evaluation of loops.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_TEMPERATURE](#)

Parameters

<code>T</code>	Temperature in centigrade
----------------	---------------------------

15.4.3.7 `double vrna_md_defaults_temperature_get (void)`

```
#include <ViennaRNA/model.h>
```

Get default temperature for energy evaluation of loops.

See also

[vrna_md_defaults_temperature\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_TEMPERATURE](#)

Returns

The global default settings for temperature in centigrade

15.4.3.8 void vrna_md_defaults_betaScale (double *b*)

```
#include <ViennaRNA/model.h>
```

Set default scaling factor of thermodynamic temperature in Boltzmann factors.

Boltzmann factors are then computed as $\exp(-E/(b \cdot kT))$.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_BETA_SCALE](#)

Parameters

<i>b</i>	The scaling factor, default is 1.0
----------	------------------------------------

15.4.3.9 double vrna_md_defaults_betaScale_get (void)

```
#include <ViennaRNA/model.h>
```

Get default scaling factor of thermodynamic temperature in Boltzmann factors.

See also

[vrna_md_defaults_betaScale\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_BETA_SCALE](#)

Returns

The global default thermodynamic temperature scaling factor

15.4.3.10 void vrna_md_defaults_dangles (int *d*)

```
#include <ViennaRNA/model.h>
```

Set default dangle model for structure prediction.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_DANGLES](#)

Parameters

<i>d</i>	The dangle model
----------	------------------

15.4.3.11 `int vrna_md_defaults_dangles_get (void)`

```
#include <ViennaRNA/model.h>
```

Get default dangle model for structure prediction.

See also

[vrna_md_defaults_dangles\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_DANGLES](#)

Returns

The global default settings for the dangle model

15.4.3.12 `void vrna_md_defaults_special_hp (int flag)`

```
#include <ViennaRNA/model.h>
```

Set default behavior for lookup of tabulated free energies for special hairpin loops, such as Tri-, Tetra-, or Hexa-loops.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_SPECIAL_HP](#)

Parameters

<i>flag</i>	On/Off switch (0 = OFF, else = ON)
-------------	------------------------------------

15.4.3.13 `int vrna_md_defaults_special_hp_get (void)`

```
#include <ViennaRNA/model.h>
```

Get default behavior for lookup of tabulated free energies for special hairpin loops, such as Tri-, Tetra-, or Hexa-loops.

See also

[vrna_md_defaults_special_hp\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_SPECIAL_HP](#)

Returns

The global default settings for the treatment of special hairpin loops

15.4.3.14 void vrna_md_defaults_noLP (int *flag*)

```
#include <ViennaRNA/model.h>
```

Set default behavior for prediction of canonical secondary structures.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_NO_LP](#)

Parameters

<i>flag</i>	On/Off switch (0 = OFF, else = ON)
-------------	------------------------------------

15.4.3.15 int vrna_md_defaults_noLP_get (void)

```
#include <ViennaRNA/model.h>
```

Get default behavior for prediction of canonical secondary structures.

See also

[vrna_md_defaults_noLP\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_NO_LP](#)

Returns

The global default settings for predicting canonical secondary structures

15.4.3.16 void vrna_md_defaults_noGU (int *flag*)

```
#include <ViennaRNA/model.h>
```

Set default behavior for treatment of G-U wobble pairs.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_NO_GU](#)

Parameters

<i>flag</i>	On/Off switch (0 = OFF, else = ON)
-------------	------------------------------------

15.4.3.17 int vrna_md_defaults_noGU_get (void)

```
#include <ViennaRNA/model.h>
```


Get default behavior for treatment of G-U wobble pairs.

See also

[vrna_md_defaults_noGU\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_NO_GU](#)

Returns

The global default settings for treatment of G-U wobble pairs

15.4.3.18 `void vrna_md_defaults_noGUclosure (int flag)`

`#include <ViennaRNA/model.h>`

Set default behavior for G-U pairs as closing pair for loops.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_NO_GU_CLOSURE](#)

Parameters

<i>flag</i>	On/Off switch (0 = OFF, else = ON)
-------------	------------------------------------

15.4.3.19 `int vrna_md_defaults_noGUclosure_get (void)`

`#include <ViennaRNA/model.h>`

Get default behavior for G-U pairs as closing pair for loops.

See also

[vrna_md_defaults_noGUclosure\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_NO_GU_CLOSURE](#)

Returns

The global default settings for treatment of G-U pairs closing a loop

15.4.3.20 `void vrna_md_defaults_logML (int flag)`

`#include <ViennaRNA/model.h>`

Set default behavior recomputing free energies of multi-branch loops using a logarithmic model.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_LOG_ML](#)

Parameters

<i>flag</i>	On/Off switch (0 = OFF, else = ON)
-------------	------------------------------------

15.4.3.21 int vrna_md_defaults_logML_get (void)

```
#include <ViennaRNA/model.h>
```

Get default behavior recomputing free energies of multi-branch loops using a logarithmic model.

See also

[vrna_md_defaults_logML\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_LOG_ML](#)

Returns

The global default settings for logarithmic model in multi-branch loop free energy evaluation

15.4.3.22 void vrna_md_defaults_circ (int *flag*)

```
#include <ViennaRNA/model.h>
```

Set default behavior whether input sequences are circularized.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_CIRC](#)

Parameters

<i>flag</i>	On/Off switch (0 = OFF, else = ON)
-------------	------------------------------------

15.4.3.23 int vrna_md_defaults_circ_get (void)

```
#include <ViennaRNA/model.h>
```

Get default behavior whether input sequences are circularized.

See also

[vrna_md_defaults_circ\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_CIRC](#)

Returns

The global default settings for treating input sequences as circular

15.4.3.24 void vrna_md_defaults_gquad (int *flag*)

```
#include <ViennaRNA/model.h>
```

Set default behavior for treatment of G-Quadruplexes.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_GQUAD](#)

Parameters

<i>flag</i>	On/Off switch (0 = OFF, else = ON)
-------------	------------------------------------

15.4.3.25 int vrna_md_defaults_gquad_get (void)

```
#include <ViennaRNA/model.h>
```

Get default behavior for treatment of G-Quadruplexes.

See also

[vrna_md_defaults_gquad\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_GQUAD](#)

Returns

The global default settings for treatment of G-Quadruplexes

15.4.3.26 void vrna_md_defaults_uniq_ML (int *flag*)

```
#include <ViennaRNA/model.h>
```

Set default behavior for creating additional matrix for unique multi-branch loop prediction.

Note

Activating this option usually results in higher memory consumption!

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_UNIQ_ML](#)

Parameters

<i>flag</i>	On/Off switch (0 = OFF, else = ON)
-------------	------------------------------------

15.4.3.27 int vrna_md_defaults_uniq_ML_get (void)

```
#include <ViennaRNA/model.h>
```

Get default behavior for creating additional matrix for unique multi-branch loop prediction.

See also

[vrna_md_defaults_uniq_ML\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_UNIQ_ML](#)

Returns

The global default settings for creating additional matrices for unique multi-branch loop prediction

15.4.3.28 void vrna_md_defaults_energy_set (int e)

```
#include <ViennaRNA/model.h>
```

Set default energy set.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_ENERGY_SET](#)

Parameters

<i>e</i>	Energy set (0, 1, 2, 3)
----------	-------------------------

15.4.3.29 int vrna_md_defaults_energy_set_get (void)

```
#include <ViennaRNA/model.h>
```

Get default energy set.

See also

[vrna_md_defaults_energy_set\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_ENERGY_SET](#)

Returns

The global default settings for the energy set

15.4.3.30 void vrna_md_defaults_backtrack (int *flag*)

```
#include <ViennaRNA/model.h>
```

Set default behavior for whether to backtrack secondary structures.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_BACKTRACK](#)

Parameters

<i>flag</i>	On/Off switch (0 = OFF, else = ON)
-------------	------------------------------------

15.4.3.31 `int vrna_md_defaults_backtrack_get (void)`

`#include <ViennaRNA/model.h>`

Get default behavior for whether to backtrack secondary structures.

See also

[vrna_md_defaults_backtrack\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_BACKTRACK](#)

Returns

The global default settings for backtracking structures

15.4.3.32 `void vrna_md_defaults_backtrack_type (char t)`

`#include <ViennaRNA/model.h>`

Set default backtrack type, i.e. which DP matrix is used.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_BACKTRACK_TYPE](#)

Parameters

<i>t</i>	The type ('F', 'C', or 'M')
----------	-----------------------------

15.4.3.33 `char vrna_md_defaults_backtrack_type_get (void)`

`#include <ViennaRNA/model.h>`

Get default backtrack type, i.e. which DP matrix is used.

See also

[vrna_md_defaults_backtrack_type\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_BACKTRACK_TYPE](#)

Returns

The global default settings that specify which DP matrix is used for backtracking

15.4.3.34 void vrna_md_defaults_compute_bpp (int *flag*)

```
#include <ViennaRNA/model.h>
```

Set the default behavior for whether to compute base pair probabilities after partition function computation.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_COMPUTE_BPP](#)

Parameters

<i>flag</i>	On/Off switch (0 = OFF, else = ON)
-------------	------------------------------------

15.4.3.35 int vrna_md_defaults_compute_bpp_get (void)

```
#include <ViennaRNA/model.h>
```

Get the default behavior for whether to compute base pair probabilities after partition function computation.

See also

[vrna_md_defaults_compute_bpp\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_COMPUTE_BPP](#)

Returns

The global default settings that specify whether base pair probabilities are computed together with partition function

15.4.3.36 void vrna_md_defaults_max_bp_span (int *span*)

```
#include <ViennaRNA/model.h>
```

Set default maximal base pair span.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_MAX_BP_SPAN](#)

Parameters

<i>span</i>	Maximal base pair span
-------------	------------------------

15.4.3.37 `int vrna_md_defaults_max_bp_span_get (void)`

```
#include <ViennaRNA/model.h>
```

Get default maximal base pair span.

See also

[vrna_md_defaults_max_bp_span\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_MAX_BP_SPAN](#)

Returns

The global default settings for maximum base pair span

15.4.3.38 `void vrna_md_defaults_min_loop_size (int size)`

```
#include <ViennaRNA/model.h>
```

Set default minimal loop size.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [TURN](#)

Parameters

<i>size</i>	Minimal size, i.e. number of unpaired nucleotides for a hairpin loop
-------------	----------------------------------------------------------------------

15.4.3.39 `int vrna_md_defaults_min_loop_size_get (void)`

```
#include <ViennaRNA/model.h>
```

Get default minimal loop size.

See also

[vrna_md_defaults_min_loop_size\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [TURN](#)

Returns

The global default settings for minimal size of hairpin loops

15.4.3.40 `void vrna_md_defaults_window_size (int size)`

```
#include <ViennaRNA/model.h>
```

Set default window size for sliding window structure prediction approaches.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_WINDOW_SIZE](#)

Parameters

<i>size</i>	The size of the sliding window
-------------	--------------------------------

15.4.3.41 `int vrna_md_defaults_window_size_get (void)`

```
#include <ViennaRNA/model.h>
```

Get default window size for sliding window structure prediction approaches.

See also

[vrna_md_defaults_window_size\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_WINDOW_SIZE](#)

Returns

The global default settings for the size of the sliding window

15.4.3.42 `void vrna_md_defaults_oldAliEn (int flag)`

```
#include <ViennaRNA/model.h>
```

Set default behavior for whether to use old energy model for comparative structure prediction.

Note

This option is outdated. Activating the old energy model usually results in worse consensus structure predictions.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_ALI_OLD_EN](#)

Parameters

<i>flag</i>	On/Off switch (0 = OFF, else = ON)
-------------	------------------------------------

15.4.3.43 `int vrna_md_defaults_oldAliEn_get (void)`

```
#include <ViennaRNA/model.h>
```

Get default behavior for whether to use old energy model for comparative structure prediction.

See also

[vrna_md_defaults_oldAliEn\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_ALI_OLD_EN](#)

Returns

The global default settings for using old energy model for comparative structure prediction

15.4.3.44 `void vrna_md_defaults_ribo (int flag)`

`#include <ViennaRNA/model.h>`

Set default behavior for whether to use Ribosum Scoring in comparative structure prediction.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_ALI_RIBO](#)

Parameters

<i>flag</i>	On/Off switch (0 = OFF, else = ON)
-------------	------------------------------------

15.4.3.45 `int vrna_md_defaults_ribo_get (void)`

`#include <ViennaRNA/model.h>`

Get default behavior for whether to use Ribosum Scoring in comparative structure prediction.

See also

[vrna_md_defaults_ribo\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_ALI_RIBO](#)

Returns

The global default settings for using Ribosum scoring in comparative structure prediction

15.4.3.46 `void vrna_md_defaults_cv_fact (double factor)`

`#include <ViennaRNA/model.h>`

Set the default co-variance scaling factor used in comparative structure prediction.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_ALI_CV_FACT](#)

Parameters

<i>factor</i>	The co-variance factor
---------------	------------------------

15.4.3.47 `double vrna_md_defaults_cv_fact_get (void)`

```
#include <ViennaRNA/model.h>
```

Get the default co-variance scaling factor used in comparative structure prediction.

See also

[vrna_md_defaults_cv_fact\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_ALI_CV_FACT](#)

Returns

The global default settings for the co-variance factor

15.4.3.48 `void vrna_md_defaults_nc_fact (double factor)`

```
#include <ViennaRNA/model.h>
```

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_ALI_NC_FACT](#)

Parameters

<i>factor</i>	
---------------	--

15.4.3.49 `double vrna_md_defaults_nc_fact_get (void)`

```
#include <ViennaRNA/model.h>
```

See also

[vrna_md_defaults_nc_fact\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#), [VRNA_MODEL_DEFAULT_ALI_NC_FACT](#)

Returns

15.4.3.50 void vrna_md_defaults_sfact (double *factor*)

```
#include <ViennaRNA/model.h>
```

Set the default scaling factor used to avoid under-/overflows in partition function computation.

See also

[vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#)

Parameters

<i>factor</i>	The scaling factor (default: 1.07)
---------------	------------------------------------

15.4.3.51 double vrna_md_defaults_sfact_get (void)

```
#include <ViennaRNA/model.h>
```

Get the default scaling factor used to avoid under-/overflows in partition function computation.

See also

[vrna_md_defaults_sfact\(\)](#), [vrna_md_defaults_reset\(\)](#), [vrna_md_set_default\(\)](#), [vrna_md_t](#)

Returns

The global default settings of the scaling factor

15.4.3.52 void set_model_details (vrna_md_t* *md*)

```
#include <ViennaRNA/model.h>
```

Set default model details.

Use this function if you wish to initialize a [vrna_md_t](#) data structure with its default values, i.e. the global model settings as provided by the deprecated global variables.

Deprecated This function will vanish as soon as backward compatibility of RNAlib is dropped (expected in version 3). Use [vrna_md_set_default\(\)](#) instead!

Parameters

<i>md</i>	A pointer to the data structure that is about to be initialized
-----------	-----------------------------------------------------------------

15.4.4 Variable Documentation

15.4.4.1 double temperature

```
#include <ViennaRNA/model.h>
```

Rescale energy parameters to a temperature in degC.

Default is 37C. You have to call the `update_..._params()` functions after changing this parameter.

Deprecated Use `vrna_md_defaults_temperature()`, and `vrna_md_defaults_temperature_get()` to change, and read the global default temperature settings

See also

`vrna_md_defaults_temperature()`, `vrna_md_defaults_temperature_get()`, `vrna_md_defaults_reset()`

15.4.4.2 double pf_scale

```
#include <ViennaRNA/model.h>
```

A scaling factor used by `pf_fold()` to avoid overflows.

Should be set to approximately $\exp((-F/kT)/length)$, where F is an estimate for the ensemble free energy, for example the minimum free energy. You must call `update_pf_params()` after changing this parameter.

If `pf_scale` is -1 (the default) , an estimate will be provided automatically when computing partition functions, e.g. `pf_fold()` The automatic estimate is usually insufficient for sequences more than a few hundred bases long.

15.4.4.3 int dangles

```
#include <ViennaRNA/model.h>
```

Switch the energy model for dangling end contributions (0, 1, 2, 3)

If set to 0 no stabilizing energies are assigned to bases adjacent to helices in free ends and multiloops (so called dangling ends). Normally (`dangles` = 1) dangling end energies are assigned only to unpaired bases and a base cannot participate simultaneously in two dangling ends. In the partition function algorithm `pf_fold()` these checks are neglected. If `dangles` is set to 2, all folding routines will follow this convention. This treatment of dangling ends gives more favorable energies to helices directly adjacent to one another, which can be beneficial since such helices often do engage in stabilizing interactions through co-axial stacking.

If `dangles` = 3 co-axial stacking is explicitly included for adjacent helices in multiloops. The option affects only mfe folding and energy evaluation (`fold()` and `energy_of_structure()`), as well as suboptimal folding (`subopt()`) via re-evaluation of energies. Co-axial stacking with one intervening mismatch is not considered so far.

Default is 2 in most algorithms, partition function algorithms can only handle 0 and 2

15.4.4.4 int tetra_loop

```
#include <ViennaRNA/model.h>
```

Include special stabilizing energies for some tri-, tetra- and hexa-loops;.

default is 1.

15.4.4.5 int noLonelyPairs

```
#include <ViennaRNA/model.h>
```

Global switch to avoid/allow helices of length 1.

Disallow all pairs which can only occur as lonely pairs (i.e. as helix of length 1). This avoids lonely base pairs in the predicted structures in most cases.

15.4.4.6 int canonicalBPonly

```
#include <ViennaRNA/model.h>
```

Do not use this variable, it will eventually be removed in one of the next versions

15.4.4.7 int energy_set

```
#include <ViennaRNA/model.h>
```

0 = BP; 1=any with GC; 2=any with AU-parameter

If set to 1 or 2: fold sequences from an artificial alphabet ABCD..., where A pairs B, C pairs D, etc. using either GC (1) or AU parameters (2); default is 0, you probably don't want to change it.

15.4.4.8 int do_backtrack

```
#include <ViennaRNA/model.h>
```

do backtracking, i.e. compute secondary structures or base pair probabilities

If 0, do not calculate pair probabilities in [pf_fold\(\)](#); this is about twice as fast. Default is 1.

15.4.4.9 char backtrack_type

```
#include <ViennaRNA/model.h>
```

A backtrack array marker for [inverse_fold\(\)](#)

If set to 'C': force (1,N) to be paired, 'M' fold as if the sequence were inside a multiloop. Otherwise ('F') the usual mfe structure is computed.

15.4.4.10 char* nonstandards

```
#include <ViennaRNA/model.h>
```

contains allowed non standard base pairs

Lists additional base pairs that will be allowed to form in addition to GC, CG, AU, UA, GU and UG. Nonstandard base pairs are given a stacking energy of 0.

15.4.4.11 int max_bp_span

```
#include <ViennaRNA/model.h>
```

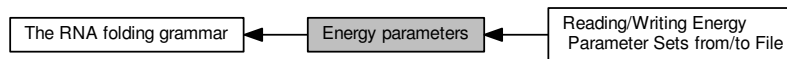
Maximum allowed base pair span.

A value of -1 indicates no restriction for distant base pairs.

15.5 Energy parameters

All relevant functions to retrieve and copy pre-calculated energy parameter sets as well as reading/writing the energy parameter set from/to file(s).

Collaboration diagram for Energy parameters:



Modules

- [Reading/Writing Energy Parameter Sets from/to File](#)
Read and Write energy parameter sets from and to text files.

Files

- file [convert_epars.h](#)
Functions and definitions for energy parameter file format conversion.
- file [energy_const.h](#)
Energy parameter constants.
- file [params.h](#)
Functions to deal with sets of energy parameters.
- file [read_epars.h](#)
Read and write energy parameter files.

Data Structures

- struct [vrna_param_s](#)
The datastructure that contains temperature scaled energy parameters. [More...](#)
- struct [vrna_exp_param_s](#)
The data structure that contains temperature scaled Boltzmann weights of the energy parameters. [More...](#)

Typedefs

- typedef struct [vrna_param_s](#) [vrna_param_t](#)
Typename for the free energy parameter data structure [vrna_params](#).
- typedef struct [vrna_exp_param_s](#) [vrna_exp_param_t](#)
Typename for the Boltzmann factor data structure [vrna_exp_params](#).
- typedef struct [vrna_param_s](#) paramT
Old typename of [vrna_param_s](#).
- typedef struct [vrna_exp_param_s](#) pf_paramT
Old typename of [vrna_exp_param_s](#).

Functions

- `vrna_param_t * vrna_params (vrna_md_t *md)`
Get a data structure containing prescaled free energy parameters.
- `vrna_param_t * vrna_params_copy (vrna_param_t *par)`
Get a copy of the provided free energy parameters.
- `vrna_exp_param_t * vrna_exp_params (vrna_md_t *md)`
Get a data structure containing prescaled free energy parameters already transformed to Boltzmann factors.
- `vrna_exp_param_t * vrna_exp_params_comparative (unsigned int n_seq, vrna_md_t *md)`
Get a data structure containing prescaled free energy parameters already transformed to Boltzmann factors (alifold version)
- `vrna_exp_param_t * vrna_exp_params_copy (vrna_exp_param_t *par)`
Get a copy of the provided free energy parameters (provided as Boltzmann factors)
- `void vrna_params_subst (vrna_fold_compound_t *vc, vrna_param_t *par)`
Update/Reset energy parameters data structure within a `vrna_fold_compound_t`.
- `void vrna_exp_params_subst (vrna_fold_compound_t *vc, vrna_exp_param_t *params)`
Update the energy parameters for subsequent partition function computations.
- `void vrna_exp_params_rescale (vrna_fold_compound_t *vc, double *mfe)`
Rescale Boltzmann factors for partition function computations.
- `void vrna_params_reset (vrna_fold_compound_t *vc, vrna_md_t *md_p)`
Reset free energy parameters within a `vrna_fold_compound_t` according to provided, or default model details.
- `void vrna_exp_params_reset (vrna_fold_compound_t *vc, vrna_md_t *md_p)`
Reset Boltzmann factors for partition function computations within a `vrna_fold_compound_t` according to provided, or default model details.
- `vrna_exp_param_t * get_scaled_pf_parameters (void)`
- `vrna_exp_param_t * get_boltzmann_factors (double temperature, double betaScale, vrna_md_t md, double pf_scale)`
Get precomputed Boltzmann factors of the loop type dependent energy contributions with independent thermodynamic temperature.
- `vrna_exp_param_t * get_boltzmann_factor_copy (vrna_exp_param_t *parameters)`
Get a copy of already precomputed Boltzmann factors.
- `vrna_exp_param_t * get_scaled_alipf_parameters (unsigned int n_seq)`
Get precomputed Boltzmann factors of the loop type dependent energy contributions (alifold variant)
- `vrna_exp_param_t * get_boltzmann_factors_ali (unsigned int n_seq, double temperature, double betaScale, vrna_md_t md, double pf_scale)`
Get precomputed Boltzmann factors of the loop type dependent energy contributions (alifold variant) with independent thermodynamic temperature.
- `vrna_param_t * scale_parameters (void)`
Get precomputed energy contributions for all the known loop types.
- `vrna_param_t * get_scaled_parameters (double temperature, vrna_md_t md)`
Get precomputed energy contributions for all the known loop types.

15.5.1 Detailed Description

All relevant functions to retrieve and copy pre-calculated energy parameter sets as well as reading/writing the energy parameter set from/to file(s).

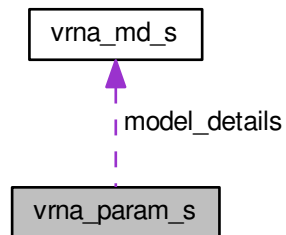
This module covers all relevant functions for pre-calculation of the energy parameters necessary for the folding routines provided by RNAlib. Furthermore, the energy parameter set in the RNAlib can be easily exchanged by a user-defined one. It is also possible to write the current energy parameter set into a text file.

15.5.2 Data Structure Documentation

15.5.2.1 struct vrna_param_s

The datastructure that contains temperature scaled energy parameters.

Collaboration diagram for vrna_param_s:



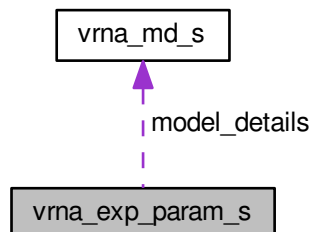
Data Fields

- double [temperature](#)
Temperature used for loop contribution scaling.
- [vrna_md_t](#) [model_details](#)
Model details to be used in the recursions.

15.5.2.2 struct vrna_exp_param_s

The data structure that contains temperature scaled Boltzmann weights of the energy parameters.

Collaboration diagram for vrna_exp_param_s:



Data Fields

- int [id](#)
An identifier for the data structure.
- double [pf_scale](#)
Scaling factor to avoid over-/underflows.
- double [temperature](#)
Temperature used for loop contribution scaling.
- double [alpha](#)
Scaling factor for the thermodynamic temperature.
- [vrna_md_t](#) [model_details](#)
Model details to be used in the recursions.

15.5.2.2.1 Field Documentation

15.5.2.2.1.1 int vrna_exp_param_s::id

An identifier for the data structure.

Deprecated This attribute will be removed in version 3

15.5.2.2.1.2 double vrna_exp_param_s::alpha

Scaling factor for the thermodynamic temperature.

This allows for temperature scaling in Boltzmann factors independently from the energy contributions. The resulting Boltzmann factors are then computed by $e^{-E/(\alpha \cdot K \cdot T)}$

15.5.3 Typedef Documentation

15.5.3.1 typedef struct vrna_param_s paramT

```
#include <ViennaRNA/params.h>
```

Old typename of [vrna_param_s](#).

Deprecated Use [vrna_param_t](#) instead!

15.5.3.2 typedef struct vrna_exp_param_s pf_paramT

```
#include <ViennaRNA/params.h>
```

Old typename of [vrna_exp_param_s](#).

Deprecated Use [vrna_exp_param_t](#) instead!

15.5.4 Function Documentation

15.5.4.1 vrna_param_t* vrna_params (vrna_md_t * md)

```
#include <ViennaRNA/params.h>
```

Get a data structure containing prescaled free energy parameters.

If a NULL pointer is passed for the model details parameter, the default model parameters are stored within the requested [vrna_param_t](#) structure.

See also

[vrna_md_t](#), [vrna_md_set_default\(\)](#), [vrna_exp_params\(\)](#)

Parameters

<i>md</i>	A pointer to the model details to store inside the structure (Maybe NULL)
-----------	---------------------------------------------------------------------------

Returns

A pointer to the memory location where the requested parameters are stored

15.5.4.2 `vrna_param_t* vrna_params_copy (vrna_param_t * par)`

```
#include <ViennaRNA/params.h>
```

Get a copy of the provided free energy parameters.

If NULL is passed as parameter, a default set of energy parameters is created and returned.

See also

[vrna_params\(\)](#), [vrna_param_t](#)

Parameters

<i>par</i>	The free energy parameters that are to be copied (Maybe NULL)
------------	---------------------------------------------------------------

Returns

A copy or a default set of the (provided) parameters

15.5.4.3 `vrna_exp_param_t* vrna_exp_params (vrna_md_t * md)`

```
#include <ViennaRNA/params.h>
```

Get a data structure containing prescaled free energy parameters already transformed to Boltzmann factors.

This function returns a data structure that contains all necessary precomputed energy contributions for each type of loop.

In contrast to [vrna_params\(\)](#), the free energies within this data structure are stored as their Boltzmann factors, i.e.

$$\exp(-E/kT)$$

where E is the free energy.

If a NULL pointer is passed for the model details parameter, the default model parameters are stored within the requested [vrna_exp_param_t](#) structure.

See also

[vrna_md_t](#), [vrna_md_set_default\(\)](#), [vrna_params\(\)](#), [vrna_rescale_pf_params\(\)](#)

Parameters

<i>md</i>	A pointer to the model details to store inside the structure (Maybe NULL)
-----------	---------------------------------------------------------------------------

Returns

A pointer to the memory location where the requested parameters are stored

15.5.4.4 `vrna_exp_param_t* vrna_exp_params_comparative (unsigned int n_seq, vrna_md_t* md)`

```
#include <ViennaRNA/params.h>
```

Get a data structure containing prescaled free energy parameters already transformed to Boltzmann factors (alifold version)

If a NULL pointer is passed for the model details parameter, the default model parameters are stored within the requested `vrna_exp_param_t` structure.

See also

`vrna_md_t`, `vrna_md_set_default()`, `vrna_exp_params()`, `vrna_params()`

Parameters

<i>n_seq</i>	The number of sequences in the alignment
<i>md</i>	A pointer to the model details to store inside the structure (Maybe NULL)

Returns

A pointer to the memory location where the requested parameters are stored

15.5.4.5 `vrna_exp_param_t* vrna_exp_params_copy (vrna_exp_param_t* par)`

```
#include <ViennaRNA/params.h>
```

Get a copy of the provided free energy parameters (provided as Boltzmann factors)

If NULL is passed as parameter, a default set of energy parameters is created and returned.

See also

`vrna_exp_params()`, `vrna_exp_param_t`

Parameters

<i>par</i>	The free energy parameters that are to be copied (Maybe NULL)
------------	---------------------------------------------------------------

Returns

A copy or a default set of the (provided) parameters

15.5.4.6 `void vrna_params_subst (vrna_fold_compound_t * vc, vrna_param_t * par)`

```
#include <ViennaRNA/params.h>
```

Update/Reset energy parameters data structure within a `vrna_fold_compound_t`.

Passing NULL as second argument leads to a reset of the energy parameters within `vc` to their default values. Otherwise, the energy parameters provided will be copied over into `vc`.

See also

`vrna_params_reset()`, `vrna_param_t`, `vrna_md_t`, `vrna_params()`

Parameters

<code>vc</code>	The <code>vrna_fold_compound_t</code> that is about to receive updated energy parameters
<code>par</code>	The energy parameters used to substitute those within <code>vc</code> (Maybe NULL)

SWIG Wrapper Notes This function is attached to `vrna_fc_s` objects as `params_subst()` method.

15.5.4.7 `void vrna_exp_params_subst (vrna_fold_compound_t * vc, vrna_exp_param_t * params)`

```
#include <ViennaRNA/params.h>
```

Update the energy parameters for subsequent partition function computations.

This function can be used to properly assign new energy parameters for partition function computations to a `vrna_fold_compound_t`. For this purpose, the data of the provided pointer `params` will be copied into `vc` and a re-computation of the partition function scaling factor is issued, if the `pf_scale` attribute of `params` is less than 1.0.

Passing NULL as second argument leads to a reset of the energy parameters within `vc` to their default values

See also

`vrna_exp_params_reset()`, `vrna_exp_params_rescale()`, `vrna_exp_param_t`, `vrna_md_t`, `vrna_exp_params()`

Parameters

<code>vc</code>	The fold compound data structure
<code>params</code>	A pointer to the new energy parameters

15.5.4.8 void vrna_exp_params_rescale (vrna_fold_compound_t * vc, double * mfe)

```
#include <ViennaRNA/params.h>
```

Rescale Boltzmann factors for partition function computations.

This function may be used to (automatically) rescale the Boltzmann factors used in partition function computations. Since partition functions over subsequences can easily become extremely large, the RNAlib internally rescales them to avoid numerical over- and/or underflow. Therefore, a proper scaling factor s needs to be chosen that in turn is then used to normalize the corresponding partition functions $\hat{q}[i, j] = q[i, j] / s^{(j-i+1)}$.

This function provides two ways to automatically adjust the scaling factor.

1. Automatic guess
2. Automatic adjustment according to MFE

Passing `NULL` as second parameter activates the *automatic guess mode*. Here, the scaling factor is recomputed according to a mean free energy of `184.3*length` cal for random sequences.

Note

This recomputation only takes place if the `pf_scale` attribute of the `exp_params` data structure contained in `vc` has a value below `1.0`.

On the other hand, if the MFE for a sequence is known, it can be used to recompute a more robust scaling factor, since it represents the lowest free energy of the entire ensemble of structures, i.e. the highest Boltzmann factor. To activate this second mode of *automatic adjustment according to MFE*, a pointer to the MFE value needs to be passed as second argument. This value is then taken to compute the scaling factor as $s = \exp((s_{fact} * MFE) / kT / length)$, where `sfact` is an additional scaling weight located in the `vrna_md_t` data structure of `exp_params` in `vc`.

The computed scaling factor s will be stored as `pf_scale` attribute of the `exp_params` data structure in `vc`.

See also

[vrna_exp_params_subst\(\)](#), [vrna_md_t](#), [vrna_exp_param_t](#), [vrna_fold_compound_t](#)

Parameters

<code>vc</code>	The fold compound data structure
<code>mfe</code>	A pointer to the MFE (in kcal/mol) or <code>NULL</code>

SWIG Wrapper Notes This function is attached to `vrna_fc_s` objects as overloaded `exp_params_rescale()` method.

When no parameter is passed to this method, the resulting action is the same as passing `NULL` as second parameter to `vrna_exp_params_rescale()`, i.e. default scaling of the partition function. Passing an energy in kcal/mol, e.g. as retrieved by a previous call to the `mfe()` method, instructs all subsequent calls to scale the partition function accordingly.

15.5.4.9 void vrna_params_reset (vrna_fold_compound_t * vc, vrna_md_t * md_p)

```
#include <ViennaRNA/params.h>
```

Reset free energy parameters within a [vrna_fold_compound_t](#) according to provided, or default model details.

This function allows one to rescale free energy parameters for subsequent structure prediction or evaluation according to a set of model details, e.g. temperature values. To do so, the caller provides either a pointer to a set of model details to be used for rescaling, or NULL if global default setting should be used.

See also

[vrna_exp_params_reset\(\)](#), [vrna_params_subs\(\)](#)

Parameters

<i>vc</i>	The fold compound data structure
<i>md_p</i>	A pointer to the new model details (or NULL for reset to defaults)

SWIG Wrapper Notes This function is attached to [vrna_fc_s](#) objects as overloaded **params_reset()** method.

When no parameter is passed to this method, the resulting action is the same as passing *NULL* as second parameter to [vrna_params_reset\(\)](#), i.e. global default model settings are used. Passing an object of type [vrna_md_s](#) resets the fold compound according to the specifications stored within the [vrna_md_s](#) object.

15.5.4.10 vrna_exp_params_reset (vrna_fold_compound_t * vc, vrna_md_t * md_p)

```
#include <ViennaRNA/params.h>
```

Reset Boltzmann factors for partition function computations within a [vrna_fold_compound_t](#) according to provided, or default model details.

This function allows one to rescale Boltzmann factors for subsequent partition function computations according to a set of model details, e.g. temperature values. To do so, the caller provides either a pointer to a set of model details to be used for rescaling, or NULL if global default setting should be used.

See also

[vrna_params_reset\(\)](#), [vrna_exp_params_subst\(\)](#), [vrna_exp_params_rescale\(\)](#)

Parameters

<i>vc</i>	The fold compound data structure
<i>md_p</i>	A pointer to the new model details (or NULL for reset to defaults)

SWIG Wrapper Notes This function is attached to [vrna_fc_s](#) objects as overloaded **exp_params_reset()** method.

When no parameter is passed to this method, the resulting action is the same as passing *NULL* as second parameter to [vrna_exp_params_reset\(\)](#), i.e. global default model settings are used. Passing an object of type [vrna_md_s](#) resets the fold compound according to the specifications stored within the [vrna_md_s](#) object.

15.5.4.11 [vrna_exp_param_t*](#) [get_scaled_pf_parameters](#) (void)

```
#include <ViennaRNA/params.h>
```

get a data structure of type [vrna_exp_param_t](#) which contains the Boltzmann weights of several energy parameters scaled according to the current temperature

Deprecated Use [vrna_exp_params\(\)](#) instead!

Returns

The data structure containing Boltzmann weights for use in partition function calculations

15.5.4.12 [vrna_exp_param_t*](#) [get_boltzmann_factors](#) (double *temperature*, double *betaScale*, [vrna_md_t](#) *md*, double *pf_scale*)

```
#include <ViennaRNA/params.h>
```

Get precomputed Boltzmann factors of the loop type dependent energy contributions with independent thermodynamic temperature.

This function returns a data structure that contains all necessary precalculated Boltzmann factors for each loop type contribution.

In contrast to [get_scaled_pf_parameters\(\)](#), this function enables setting of independent temperatures for both, the individual energy contributions as well as the thermodynamic temperature used in $\exp(-\Delta G/kT)$

Deprecated Use [vrna_exp_params\(\)](#) instead!

See also

[get_scaled_pf_parameters\(\)](#), [get_boltzmann_factor_copy\(\)](#)

Parameters

<i>temperature</i>	The temperature in degrees Celcius used for (re-)scaling the energy contributions
<i>betaScale</i>	A scaling value that is used as a multiplication factor for the absolute temperature of the system
<i>md</i>	The model details to be used
<i>pf_scale</i>	The scaling factor for the Boltzmann factors

Returns

A set of precomputed Boltzmann factors

15.5.4.13 `vrna_exp_param_t* get_boltzmann_factor_copy (vrna_exp_param_t* parameters)`

```
#include <ViennaRNA/params.h>
```

Get a copy of already precomputed Boltzmann factors.

Deprecated Use `vrna_exp_params_copy()` instead!

See also

`get_boltzmann_factors()`, `get_scaled_pf_parameters()`

Parameters

<i>parameters</i>	The input data structure that shall be copied
-------------------	-----------------------------------------------

Returns

A copy of the provided Boltzmann factor data set

15.5.4.14 `vrna_exp_param_t* get_scaled_alipf_parameters (unsigned int n_seq)`

```
#include <ViennaRNA/params.h>
```

Get precomputed Boltzmann factors of the loop type dependent energy contributions (alifold variant)

Deprecated Use `vrna_exp_params_comparative()` instead!

15.5.4.15 `vrna_exp_param_t* get_boltzmann_factors_ali (unsigned int n_seq, double temperature, double betaScale, vrna_md_t md, double pf_scale)`

```
#include <ViennaRNA/params.h>
```

Get precomputed Boltzmann factors of the loop type dependent energy contributions (alifold variant) with independent thermodynamic temperature.

Deprecated Use `vrna_exp_params_comparative()` instead!

15.5.4.16 `vrna_param_t*` `scale_parameters (void)`

```
#include <ViennaRNA/params.h>
```

Get precomputed energy contributions for all the known loop types.

Note

OpenMP: This function relies on several global model settings variables and thus is not to be considered threadsafe. See [get_scaled_parameters\(\)](#) for a completely threadsafe implementation.

Deprecated Use [vrna_params\(\)](#) instead!

Returns

A set of precomputed energy contributions

15.5.4.17 `vrna_param_t*` `get_scaled_parameters (double temperature, vrna_md_t md)`

```
#include <ViennaRNA/params.h>
```

Get precomputed energy contributions for all the known loop types.

Call this function to retrieve precomputed energy contributions, i.e. scaled according to the temperature passed. Furthermore, this function assumes a data structure that contains the model details as well, such that subsequent folding recursions are able to retrieve the correct model settings

Deprecated Use [vrna_params\(\)](#) instead!

See also

[vrna_md_t](#), [set_model_details\(\)](#)

Parameters

<i>temperature</i>	The temperature in degrees Celcius
<i>md</i>	The model details

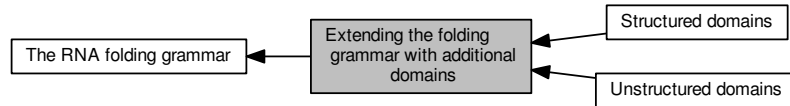
Returns

precomputed energy contributions and model settings

15.6 Extending the folding grammar with additional domains

This module covers simple and straight-forward extensions to the RNA folding grammar.

Collaboration diagram for Extending the folding grammar with additional domains:



Modules

- [Unstructured domains](#)

Add and modify unstructured domains to the RNA folding grammar.

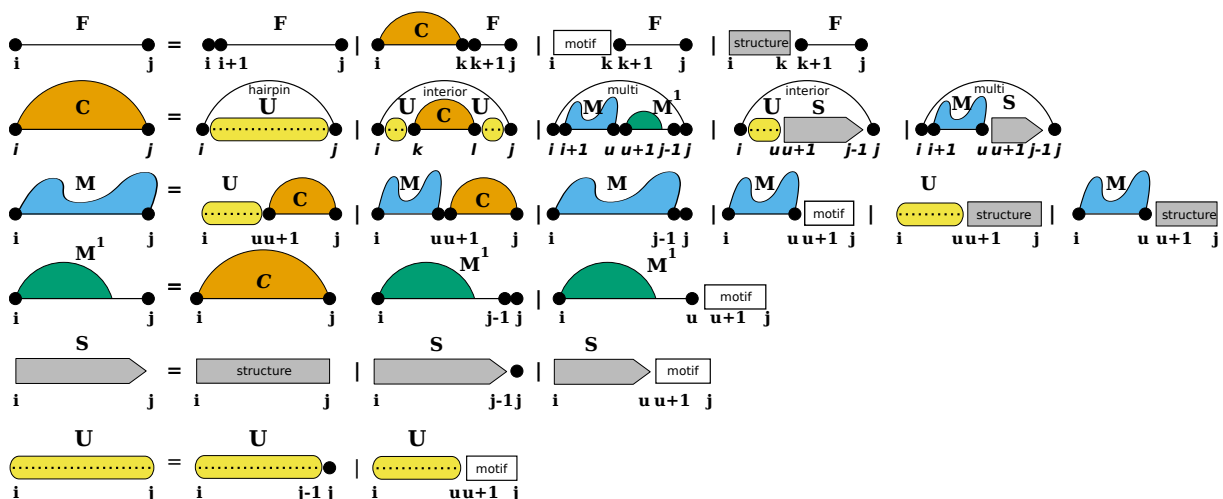
- [Structured domains](#)

Add and modify structured domains to the RNA folding grammar.

15.6.1 Detailed Description

This module covers simple and straight-forward extensions to the RNA folding grammar.

Some applications of RNA secondary structure prediction require an extension of the *regular* RNA folding grammar. For instance one would like to include proteins and other ligands binding to unpaired loop regions while competing with conventional base pairing. Another application could be that one may want to include the formation of self-enclosed structural modules, such as G-quadruplexes. For such applications, we provide a pair of additional domains that extend the regular RNA folding grammar, [Structured domains](#) and [Unstructured domains](#).



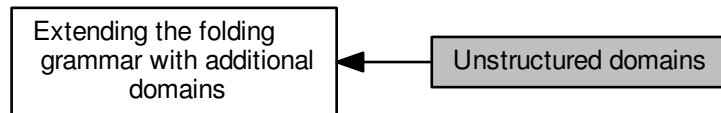
While unstructured domains are usually determined by a more or less precise sequence motif, e.g. the binding site for a protein, structured domains are considered self-enclosed modules with a more or less complex pairing pattern. Our extension with these two domains introduces two production rules to fill additional dynamic programming matrices S and U where we store the pre-computed contributions of structured domains (S), and unstructured domains (U).

For the sake of flexibility, each of the domains is associated with a specific data structure serving as an abstract interface to the extension. The interface uses callback functions to (i) pre-compute arbitrary data, e.g. filling up additional dynamic programming matrices, and (ii) evaluate the contribution of a paired or unpaired structural feature of the RNA. Implementations of these callbacks are separate for regular free energy evaluation, e.g. MFE prediction, and partition function applications. A data structure holding arbitrary data required for the callback functions can be associated to the domain as well. While RNAlib comes with a default implementation for structured and unstructured domains, the system is entirely user-customizable.

15.7 Unstructured domains

Add and modify unstructured domains to the RNA folding grammar.

Collaboration diagram for Unstructured domains:



Files

- file [unstructured_domains.h](#)

Functions to modify unstructured domains, e.g. to incorporate ligands binding to unpaired stretches.

Data Structures

- struct [vrna_unstructured_domain_s](#)

Data structure to store all functionality for ligand binding. [More...](#)

Macros

- `#define VRNA_UNSTRUCTURED_DOMAIN_EXT_LOOP 1U`
Flag to indicate ligand bound to unpaired stretch in the exterior loop.
- `#define VRNA_UNSTRUCTURED_DOMAIN_HP_LOOP 2U`
Flag to indicate ligand bound to unpaired stretch in a hairpin loop.
- `#define VRNA_UNSTRUCTURED_DOMAIN_INT_LOOP 4U`
Flag to indicate ligand bound to unpaired stretch in an interior loop.
- `#define VRNA_UNSTRUCTURED_DOMAIN_MB_LOOP 8U`
Flag to indicate ligand bound to unpaired stretch in a multibranch loop.
- `#define VRNA_UNSTRUCTURED_DOMAIN_MOTIF 16U`
Flag to indicate ligand binding without additional unbound nucleotides (motif-only)
- `#define VRNA_UNSTRUCTURED_DOMAIN_ALL_LOOPS (VRNA_UNSTRUCTURED_DOMAIN_EXT_LOOP | VRNA_UNSTRUCTURED_DOMAIN_HP_LOOP | VRNA_UNSTRUCTURED_DOMAIN_INT_LOOP | VRNA_UNSTRUCTURED_DOMAIN_MB_LOOP)`
Flag to indicate ligand bound to unpaired stretch in any loop (convenience macro)

Typedefs

- typedef struct [vrna_unstructured_domain_s](#) [vrna_ud_t](#)
Typename for the ligand binding extension data structure [vrna_unstructured_domain_s](#).
- typedef int([vrna_callback_ud_energy](#)) ([vrna_fold_compound_t](#) *vc, int i, int j, unsigned int loop_type, void *data)
Callback to retrieve binding free energy of a ligand bound to an unpaired sequence segment.
- typedef [FLT_OR_DBL](#)([vrna_callback_ud_exp_energy](#)) ([vrna_fold_compound_t](#) *vc, int i, int j, unsigned int loop_type, void *data)
Callback to retrieve Boltzmann factor of the binding free energy of a ligand bound to an unpaired sequence segment.
- typedef void([vrna_callback_ud_production](#)) ([vrna_fold_compound_t](#) *vc, void *data)
Callback for pre-processing the production rule of the ligand binding to unpaired stretches feature.
- typedef void([vrna_callback_ud_exp_production](#)) ([vrna_fold_compound_t](#) *vc, void *data)
Callback for pre-processing the production rule of the ligand binding to unpaired stretches feature (partition function variant)
- typedef void([vrna_callback_ud_probs_add](#)) ([vrna_fold_compound_t](#) *vc, int i, int j, unsigned int loop_type, [FLT_OR_DBL](#) exp_energy, void *data)
Callback to store/add equilibrium probability for a ligand bound to an unpaired sequence segment.
- typedef [FLT_OR_DBL](#)([vrna_callback_ud_probs_get](#)) ([vrna_fold_compound_t](#) *vc, int i, int j, unsigned int loop_type, int motif, void *data)
Callback to retrieve equilibrium probability for a ligand bound to an unpaired sequence segment.

Functions

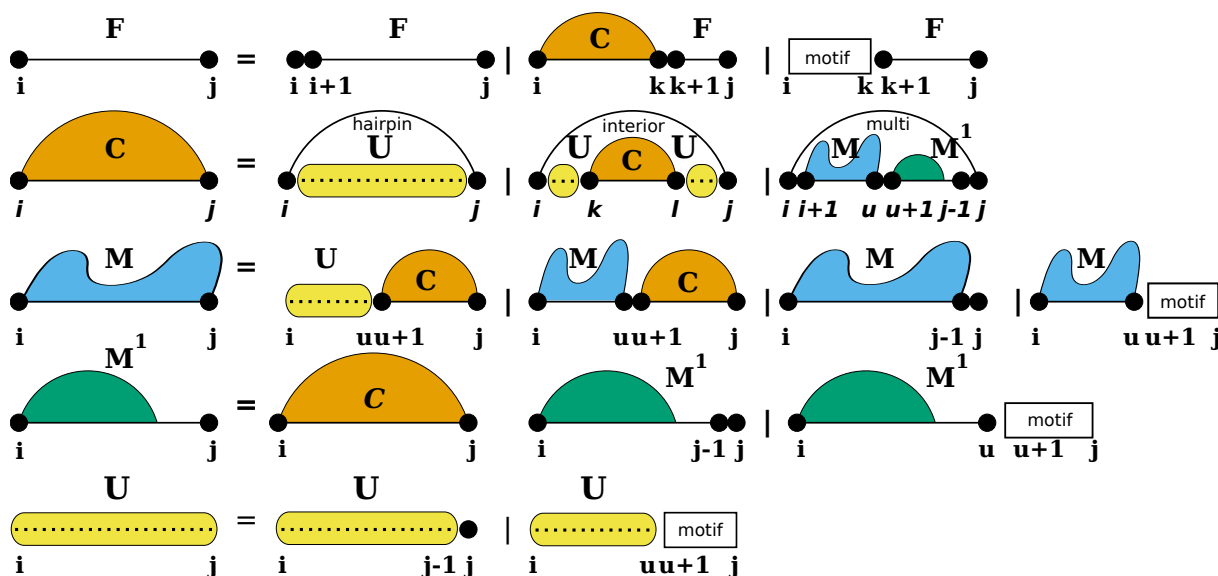
- void [vrna_ud_add_motif](#) ([vrna_fold_compound_t](#) *vc, const char *motif, double motif_en, unsigned int loop_type)
Add an unstructured domain motif, e.g. for ligand binding.
- void [vrna_ud_remove](#) ([vrna_fold_compound_t](#) *vc)
Remove ligand binding to unpaired stretches.
- void [vrna_ud_set_data](#) ([vrna_fold_compound_t](#) *vc, void *data, [vrna_callback_free_auxdata](#) *free_cb)
Attach an auxiliary data structure.
- void [vrna_ud_set_prod_rule_cb](#) ([vrna_fold_compound_t](#) *vc, [vrna_callback_ud_production](#) *pre_cb, [vrna_callback_ud_energy](#) *e_cb)
Attach production rule callbacks for free energies computations.
- void [vrna_ud_set_exp_prod_rule_cb](#) ([vrna_fold_compound_t](#) *vc, [vrna_callback_ud_exp_production](#) *pre_cb, [vrna_callback_ud_exp_energy](#) *exp_e_cb)
Attach production rule for partition function.

15.7.1 Detailed Description

Add and modify unstructured domains to the RNA folding grammar.

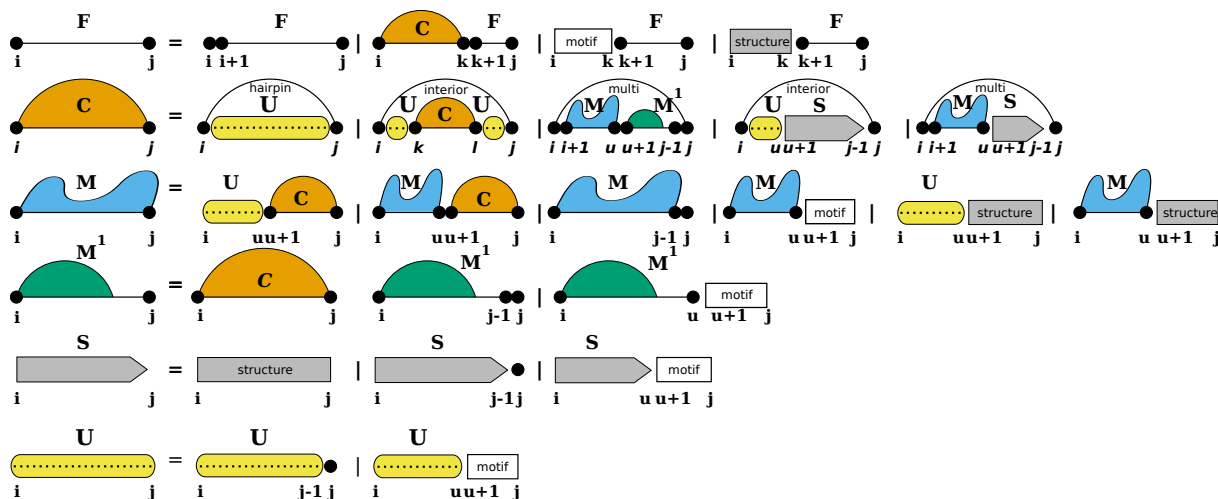
This module provides the tools to add and modify unstructured domains to the production rules of the RNA folding grammar. Usually this functionality is utilized for incorporating ligand binding to unpaired stretches of an RNA.

Unstructured domains appear in the production rules of the RNA folding grammar wherever new unpaired nucleotides are attached to a growing substructure (see also [12]):



The white boxes represent the stretch of RNA bound to the ligand and represented by a more or less specific sequence motif. The motif itself is considered unable to form basepairs. The additional production rule *U* is used to precompute the contribution of unpaired stretches possibly bound by one or more ligands. The auxiliary DP matrix for this production rule is filled right before processing the other (regular) production rules of the RNA folding grammar.

In a context with [Structured domains](#) the grammar is extended as follows:



Bug Although the additional production rule(s) for unstructured domains in the descriptions of this feature are always treated as 'segments possibly bound to one or more ligands', the current implementation requires that at least one ligand is bound. The default implementation already takes care of the required changes, however, upon using callback functions other than the default ones, one has to take care of this fact. Please also note, that this behavior might change in one of the next releases, such that the decomposition schemes as shown above comply with the actual implementation.

A default implementation allows one to readily use this feature by simply adding sequence motifs and corresponding binding free energies with the function `vrna_ud_add_motif()` (see also [Ligands binding to unstructured domains](#)).

The grammar extension is realized using a callback function that

- evaluates the binding free energy of a ligand to its target sequence segment (white boxes in the figures above), or
- returns the free energy of an unpaired stretch possibly bound by a ligand, stored in the additional U DP matrix.

The callback is passed the segment positions, the loop context, and which of the two above mentioned evaluations are required. A second callback implements the pre-processing step that prepares the U DP matrix by evaluating all possible cases of the additional production rule. Both callbacks have a default implementation in *RNAlib*, but may be over-written by a user-implementation, making it fully user-customizable.

For equilibrium probability computations, two additional callbacks exist. One to store/add and one to retrieve the probability of unstructured domains at particular positions. Our implementation already takes care of computing the probabilities, but users of the unstructured domain feature are required to provide a mechanism to efficiently store/add the corresponding values into some external data structure.

15.7.2 Data Structure Documentation

15.7.2.1 struct vrna_unstructured_domain_s

Data structure to store all functionality for ligand binding.

Data Fields

- int `uniq_motif_count`
The unique number of motifs of different lengths.
- unsigned int * `uniq_motif_size`
An array storing a unique list of motif lengths.
- int `motif_count`
Total number of distinguished motifs.
- char ** `motif`
Motif sequences.
- unsigned int * `motif_size`
Motif lengths.
- double * `motif_en`
Ligand binding free energy contribution.
- unsigned int * `motif_type`
Type of motif, i.e. loop type the ligand binds to.
- `vrna_callback_ud_production` * `prod_cb`
Callback to ligand binding production rule, i.e. create/fill DP free energy matrices.
- `vrna_callback_ud_exp_production` * `exp_prod_cb`
Callback to ligand binding production rule, i.e. create/fill DP partition function matrices.
- `vrna_callback_ud_energy` * `energy_cb`
Callback to evaluate free energy of ligand binding to a particular unpaired stretch.
- `vrna_callback_ud_exp_energy` * `exp_energy_cb`
Callback to evaluate Boltzmann factor of ligand binding to a particular unpaired stretch.
- void * `data`
Auxiliary data structure passed to energy evaluation callbacks.
- `vrna_callback_free_auxdata` * `free_data`
Callback to free auxiliary data structure.
- `vrna_callback_ud_probs_add` * `probs_add`
Callback to store/add outside partition function.
- `vrna_callback_ud_probs_get` * `probs_get`
Callback to retrieve outside partition function.

15.7.2.1.1 Field Documentation

15.7.2.1.1.1 `vrna_callback_ud_production* vrna_unstructured_domain_s::prod_cb`

Callback to ligand binding production rule, i.e. create/fill DP free energy matrices.

This callback will be executed right before the actual secondary structure decompositions, and, therefore, any implementation must not interleave with the regular DP matrices.

15.7.3 Function Documentation

15.7.3.1 `void vrna_ud_add_motif (vrna_fold_compound_t * vc, const char * motif, double motif_en, unsigned int loop_type)`

```
#include <ViennaRNA/unstructured_domains.h>
```

Add an unstructured domain motif, e.g. for ligand binding.

This function adds a ligand binding motif and the associated binding free energy to the `vrna_ud_t` attribute of a `vrna_fold_compound_t`. The motif data will then be used in subsequent secondary structure predictions. Multiple calls to this function with different motifs append all additional data to a list of ligands, which all will be evaluated. Ligand motif data can be removed from the `vrna_fold_compound_t` again using the `vrna_ud_remove()` function. The loop type parameter allows one to limit the ligand binding to particular loop type, such as the exterior loop, hairpin loops, interior loops, or multibranch loops.

See also

`VRNA_UNSTRUCTURED_DOMAIN_EXT_LOOP`, `VRNA_UNSTRUCTURED_DOMAIN_HP_LOOP`, `VRNA_UNSTRUCTURED_DOMAIN_INT_LOOP`, `VRNA_UNSTRUCTURED_DOMAIN_MB_LOOP`, `VRNA_UNSTRUCTURED_DOMAIN_ALL_LOOPS`, `vrna_ud_remove()`

Parameters

<code>vc</code>	The <code>vrna_fold_compound_t</code> data structure the ligand motif should be bound to
<code>motif</code>	The sequence motif the ligand binds to
<code>motif_en</code>	The binding free energy of the ligand in kcal/mol
<code>loop_type</code>	The loop type the ligand binds to

SWIG Wrapper Notes This function is attached as method `ud_add_motif()` to objects of type `fold_compound`

15.7.3.2 `void vrna_ud_remove (vrna_fold_compound_t * vc)`

```
#include <ViennaRNA/unstructured_domains.h>
```

Remove ligand binding to unpaired stretches.

This function removes all ligand motifs that were bound to a `vrna_fold_compound_t` using the `vrna_ud_add_motif()` function.

Parameters

vc	The vrna_fold_compound_t data structure the ligand motif data should be removed from
----	------------------------------------------------------------------------------------------------------

SWIG Wrapper Notes This function is attached as method **ud_remove()** to objects of type *fold_compound*

15.7.3.3 void vrna_ud_set_data (vrna_fold_compound_t * vc, void * data, vrna_callback_free_auxdata * free)

```
#include <ViennaRNA/unstructured_domains.h>
```

Attach an auxiliary data structure.

This function binds an arbitrary, auxiliary data structure for user-implemented ligand binding. The optional callback *free* will be passed the bound data structure whenever the [vrna_fold_compound_t](#) is removed from memory to avoid memory leaks.

See also

[vrna_ud_set_prod_rule_cb\(\)](#), [vrna_ud_set_exp_prod_rule_cb\(\)](#), [vrna_ud_remove\(\)](#)

Parameters

vc	The vrna_fold_compound_t data structure the auxiliary data structure should be bound to
data	A pointer to the auxiliary data structure
free_cb	A pointer to a callback function that free's memory occupied by <i>data</i>

SWIG Wrapper Notes This function is attached as method **ud_set_data()** to objects of type *fold_compound*

15.7.3.4 void vrna_ud_set_prod_rule_cb (vrna_fold_compound_t * vc, vrna_callback_ud_production * pre_cb, vrna_callback_ud_energy * e_cb)

```
#include <ViennaRNA/unstructured_domains.h>
```

Attach production rule callbacks for free energies computations.

Use this function to bind a user-implemented grammar extension for unstructured domains.

The callback *e_cb* needs to evaluate the free energy contribution $f(i, j)$ of the unpaired segment $[i, j]$. It will be executed in each of the regular secondary structure production rules. Whenever the callback is passed the [VRNA_UNSTRUCTURED_DOMAIN_MOTIF](#) flag via its *loop_type* parameter the contribution of any ligand that consecutively binds from position *i* to *j* (the white box) is requested. Otherwise, the callback usually performs a lookup in the precomputed *B* matrices. Which *B* matrix is addressed will be indicated by the flags [VRNA_UNSTRUCTURED_DOMAIN_EXT_LOOP](#), [VRNA_UNSTRUCTURED_DOMAIN_HP_LOOP](#), [VRNA_UNSTRUCTURED_DOMAIN_INT_LOOP](#), and [VRNA_UNSTRUCTURED_DOMAIN_MB_LOOP](#). As their names already imply, they specify exterior loops (*E* production rule), hairpin loops and interior loops (*C* production rule), and multibranch loops (*M* and *M1* production rule).

$$f(i,j) = \boxed{} \mid \overbrace{}^B $$

i *j* *i* *j*

The `pre_cb` callback will be executed as a pre-processing step right before the regular secondary structure rules. Usually one would use this callback to fill the dynamic programming matrices \mathbb{U} and preparations of the auxiliary data structure [vrna_unstructured_domain_s.data](#)

$$\overbrace{}^B = \overbrace{}^B \bullet \mid \overbrace{}^B \boxed{}$$

i *j* *i* *j-1* *j* *i* *u* *u+1* *j*

Parameters

<code>vc</code>	The vrna_fold_compound_t data structure the callback will be bound to
<code>pre_cb</code>	A pointer to a callback function for the \mathbb{B} production rule
<code>e_cb</code>	A pointer to a callback function for free energy evaluation

SWIG Wrapper Notes This function is attached as method `ud_set_prod_rule_cb()` to objects of type `fold_↔compound`

15.7.3.5 `void vrna_ud_set_exp_prod_rule_cb(vrna_fold_compound_t * vc, vrna_callback_ud_exp_production * pre_cb, vrna_callback_ud_exp_energy * exp_e_cb)`

```
#include <ViennaRNA/unstructured_domains.h>
```

Attach production rule for partition function.

This function is the partition function companion of [vrna_ud_set_prod_rule_cb\(\)](#).

Use it to bind callbacks to (i) fill the \mathbb{U} production rule dynamic programming matrices and/or prepare the [vrna_↔unstructured_domain_s.data](#), and (ii) provide a callback to retrieve partition functions for subsegments $[i, j]$.

$$\overbrace{}^B = \overbrace{}^B \bullet \mid \overbrace{}^B \boxed{}$$

i *j* *i* *j-1* *j* *i* *u* *u+1* *j*

$$f(i,j) = \boxed{} \mid \overbrace{}^B$$

i *j* *i* *j*

See also

[vrna_ud_set_prod_rule_cb\(\)](#)

Parameters

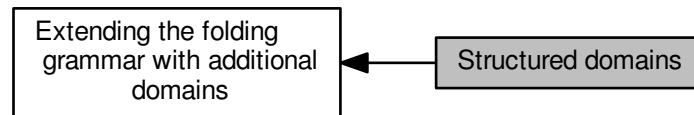
<i>vc</i>	The vrna_fold_compound_t data structure the callback will be bound to
<i>pre_cb</i>	A pointer to a callback function for the \mathbb{B} production rule
<i>exp_e_cb</i>	A pointer to a callback function that retrieves the partition function for a segment $[i, j]$ that may be bound by one or more ligands.

SWIG Wrapper Notes This function is attached as method `ud_set_exp_prod_rule_cb()` to objects of type `fold↔_compound`

15.8 Structured domains

Add and modify structured domains to the RNA folding grammar.

Collaboration diagram for Structured domains:



Files

- file [structured_domains.h](#)

This module provides interfaces that deal with additional structured domains in the folding grammar.

15.8.1 Detailed Description

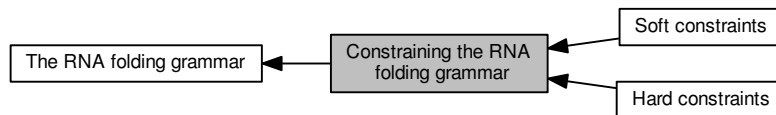
Add and modify structured domains to the RNA folding grammar.

This module provides the tools to add and modify structured domains to the production rules of the RNA folding grammar. Usually this functionality is utilized for incorporating self-enclosed structural modules that exhibit a more or less complex base pairing pattern.

15.9 Constraining the RNA folding grammar

This module provides general functions that allow for an easy control of constrained secondary structure prediction and evaluation.

Collaboration diagram for Constraining the RNA folding grammar:



Modules

- [Hard constraints](#)
This module covers all functionality for hard constraints in secondary structure prediction.
- [Soft constraints](#)
Functions and data structures for secondary structure soft constraints.

Files

- file [constraints.h](#)
Functions and data structures for constraining secondary structure predictions and evaluation.

Macros

- `#define VRNA_CONSTRAINT_FILE 0`
Flag for [vrna_constraints_add\(\)](#) to indicate that constraints are present in a text file.
- `#define VRNA_CONSTRAINT_SOFT_MFE 0`
Indicate generation of constraints for MFE folding.
- `#define VRNA_CONSTRAINT_SOFT_PF VRNA_OPTION_PF`
Indicate generation of constraints for partition function computation.
- `#define VRNA_DECOMP_PAIR_HP 1`
Flag passed to generic softt constraints callback to indicate hairpin loop decomposition step.
- `#define VRNA_DECOMP_PAIR_IL 2`
Indicator for interior loop decomposition step.
- `#define VRNA_DECOMP_PAIR_ML 3`
Indicator for multibranch loop decomposition step.
- `#define VRNA_DECOMP_ML_ML_ML 5`
Indicator for decomposition of multibranch loop part.
- `#define VRNA_DECOMP_ML_STEM 4`
Indicator for decomposition of multibranch loop part.
- `#define VRNA_DECOMP_ML_ML 6`
Indicator for decomposition of multibranch loop part.
- `#define VRNA_DECOMP_ML_UP 11`

- Indicator for decomposition of multibranch loop part.*
- `#define VRNA_DECOMP_ML_ML_STEM 20`
- Indicator for decomposition of multibranch loop part.*
- `#define VRNA_DECOMP_ML_COAXIAL 13`
- Indicator for decomposition of multibranch loop part.*
- `#define VRNA_DECOMP_EXT_EXT 9`
- Indicator for decomposition of exterior loop part.*
- `#define VRNA_DECOMP_EXT_UP 8`
- Indicator for decomposition of exterior loop part.*
- `#define VRNA_DECOMP_EXT_STEM 14`
- Indicator for decomposition of exterior loop part.*
- `#define VRNA_DECOMP_EXT_EXT_EXT 15`
- Indicator for decomposition of exterior loop part.*
- `#define VRNA_DECOMP_EXT_STEM_EXT 16`
- Indicator for decomposition of exterior loop part.*
- `#define VRNA_DECOMP_EXT_STEM_OUTSIDE 17`
- Indicator for decomposition of exterior loop part.*
- `#define VRNA_DECOMP_EXT_EXT_STEM 18`
- Indicator for decomposition of exterior loop part.*
- `#define VRNA_DECOMP_EXT_EXT_STEM1 19`
- Indicator for decomposition of exterior loop part.*

Functions

- void `vrna_constraints_add` (`vrna_fold_compound_t` *vc, const char *constraint, unsigned int options)
Add constraints to a `vrna_fold_compound_t` data structure.
- void `vrna_message_constraint_options` (unsigned int option)
Print a help message for pseudo dot-bracket structure constraint characters to stdout. (constraint support is specified by option parameter)
- void `vrna_message_constraint_options_all` (void)
Print structure constraint characters to stdout (full constraint support)

15.9.1 Detailed Description

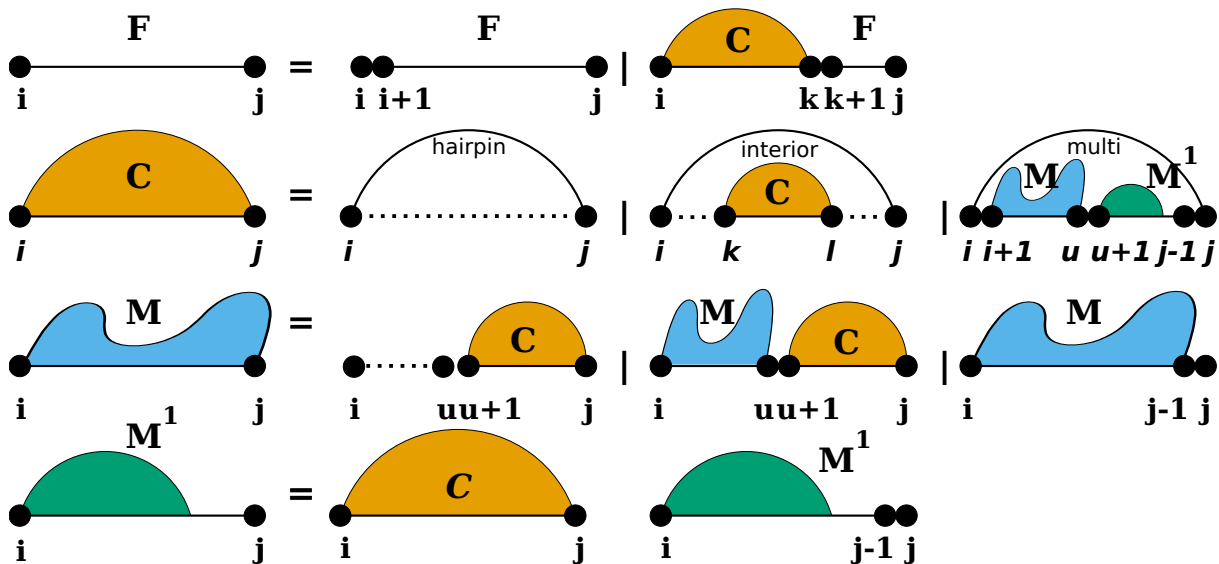
This module provides general functions that allow for an easy control of constrained secondary structure prediction and evaluation.

Secondary Structure constraints can be subdivided into two groups:

- [Hard constraints](#), and
- [Soft constraints](#).

While Hard-Constraints directly influence the production rules used in the folding recursions by allowing, disallowing, or enforcing certain decomposition steps, Soft-constraints on the other hand are used to change position specific contributions in the recursions by adding bonuses/penalties in form of pseudo free energies to certain loop configurations.

Secondary structure constraints are always applied at decomposition level, i.e. in each step of the recursive structure decomposition, for instance during MFE prediction. Below is a visualization of the decomposition scheme



For [Hard constraints](#) the following option flags may be used to constrain the pairing behavior of single, or pairs of nucleotides:

- [VRNA_CONSTRAINT_CONTEXT_EXT_LOOP](#) - Hard constraints flag, base pair in the exterior loop.
- [VRNA_CONSTRAINT_CONTEXT_HP_LOOP](#) - Hard constraints flag, base pair encloses hairpin loop.
- [VRNA_CONSTRAINT_CONTEXT_INT_LOOP](#) - Hard constraints flag, base pair encloses an interior loop.
- [VRNA_CONSTRAINT_CONTEXT_INT_LOOP_ENC](#) - Hard constraints flag, base pair encloses a multi branch loop.
- [VRNA_CONSTRAINT_CONTEXT_MB_LOOP](#) - Hard constraints flag, base pair is enclosed in an interior loop.
- [VRNA_CONSTRAINT_CONTEXT_MB_LOOP_ENC](#) - Hard constraints flag, base pair is enclosed in a multi branch loop.
- [VRNA_CONSTRAINT_CONTEXT_ENFORCE](#) - Hard constraint flag to indicate enforcement of constraints.
- [VRNA_CONSTRAINT_CONTEXT_NO_REMOVE](#) - Hard constraint flag to indicate not to remove base pairs that conflict with a given constraint.
- [VRNA_CONSTRAINT_CONTEXT_ALL_LOOPS](#) - Hard constraints flag, shortcut for all base pairs.

However, for [Soft constraints](#) we do not allow for simple loop type dependent constraining. But soft constraints are equipped with generic constraint support. This enables the user to pass arbitrary callback functions that return auxiliary energy contributions for evaluation the evaluation of any decomposition.

The callback will then always be notified about the type of decomposition that is happening, and the corresponding delimiting sequence positions. The following decomposition steps are distinguished, and should be captured by the user's implementation of the callback:

- [VRNA_DECOMP_PAIR_HP](#) - Flag passed to generic softt constraints callback to indicate hairpin loop decomposition step.
- [VRNA_DECOMP_PAIR_IL](#) - Indicator for interior loop decomposition step.
- [VRNA_DECOMP_PAIR_ML](#) - Indicator for multibranch loop decomposition step.
- [VRNA_DECOMP_ML_ML_ML](#) - Indicator for decomposition of multibranch loop part.

- [VRNA_DECOMP_ML_STEM](#) - Indicator for decomposition of multibranch loop part.
- [VRNA_DECOMP_ML_ML](#) - Indicator for decomposition of multibranch loop part.
- [VRNA_DECOMP_ML_UP](#) - Indicator for decomposition of multibranch loop part.
- [VRNA_DECOMP_ML_ML_STEM](#) - Indicator for decomposition of multibranch loop part.
- [VRNA_DECOMP_ML_COAXIAL](#) - Indicator for decomposition of multibranch loop part.
- [VRNA_DECOMP_EXT_EXT](#) - Indicator for decomposition of exterior loop part.
- [VRNA_DECOMP_EXT_UP](#) - Indicator for decomposition of exterior loop part.
- [VRNA_DECOMP_EXT_STEM](#) - Indicator for decomposition of exterior loop part.
- [VRNA_DECOMP_EXT_EXT_EXT](#) - Indicator for decomposition of exterior loop part.
- [VRNA_DECOMP_EXT_STEM_EXT](#) - Indicator for decomposition of exterior loop part.
- [VRNA_DECOMP_EXT_STEM_OUTSIDE](#) - Indicator for decomposition of exterior loop part.
- [VRNA_DECOMP_EXT_EXT_STEM](#) - Indicator for decomposition of exterior loop part.
- [VRNA_DECOMP_EXT_EXT_STEM1](#) - Indicator for decomposition of exterior loop part.

Simplified interfaces to the soft constraints framework can be obtained by the implementations in the submodules

- [SHAPE reactivity data](#) and
- ligands.

An implementation that generates soft constraints for unpaired nucleotides by minimizing the discrepancy between their predicted and expected pairing probability is available in submodule [Generate soft constraints from data](#).

15.9.2 Macro Definition Documentation

15.9.2.1 `#define VRNA_CONSTRAINT_FILE 0`

```
#include <ViennaRNA/constraints.h>
```

Flag for [vrna_constraints_add\(\)](#) to indicate that constraints are present in a text file.

See also

[vrna_constraints_add\(\)](#)

Deprecated Use 0 instead!

15.9.2.2 `#define VRNA_CONSTRAINT_SOFT_MFE 0`

```
#include <ViennaRNA/constraints.h>
```

Indicate generation of constraints for MFE folding.

Deprecated This flag has no meaning anymore, since constraints are now always stored!

15.9.2.3 `#define VRNA_CONSTRAINT_SOFT_PF VRNA_OPTION_PF`

```
#include <ViennaRNA/constraints.h>
```

Indicate generation of constraints for partition function computation.

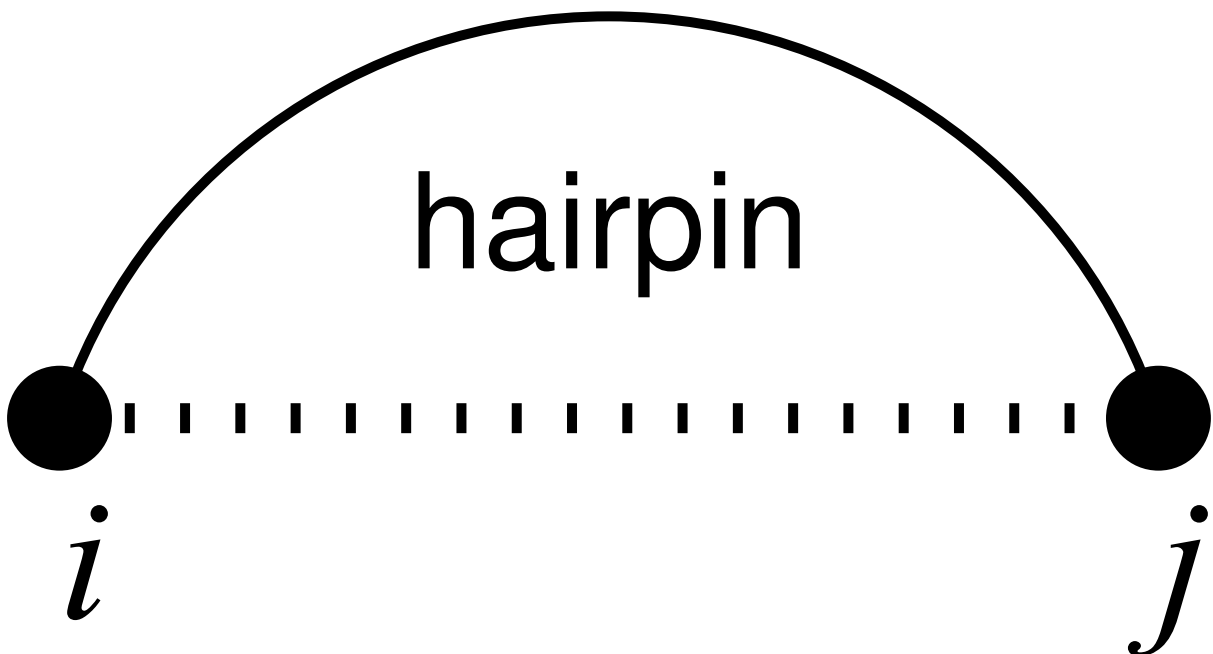
Deprecated Use `VRNA_OPTION_PF` instead!

15.9.2.4 `#define VRNA_DECOMP_PAIR_HP 1`

```
#include <ViennaRNA/constraints.h>
```

Flag passed to generic softt constraints callback to indicate hairpin loop decomposition step.

This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates a hairpin loop enclosed by the base pair (i, j) .

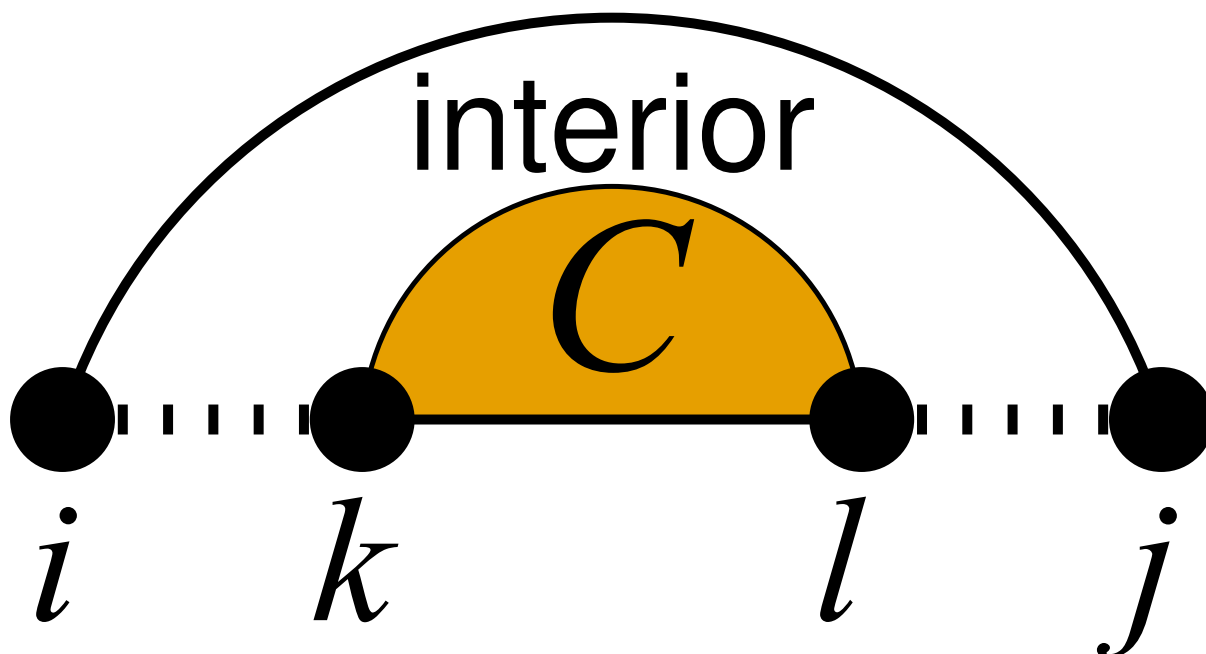


15.9.2.5 `#define VRNA_DECOMP_PAIR_IL 2`

```
#include <ViennaRNA/constraints.h>
```

Indicator for interior loop decomposition step.

This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates an interior loop enclosed by the base pair (i, j) , and enclosing the base pair (k, l) .

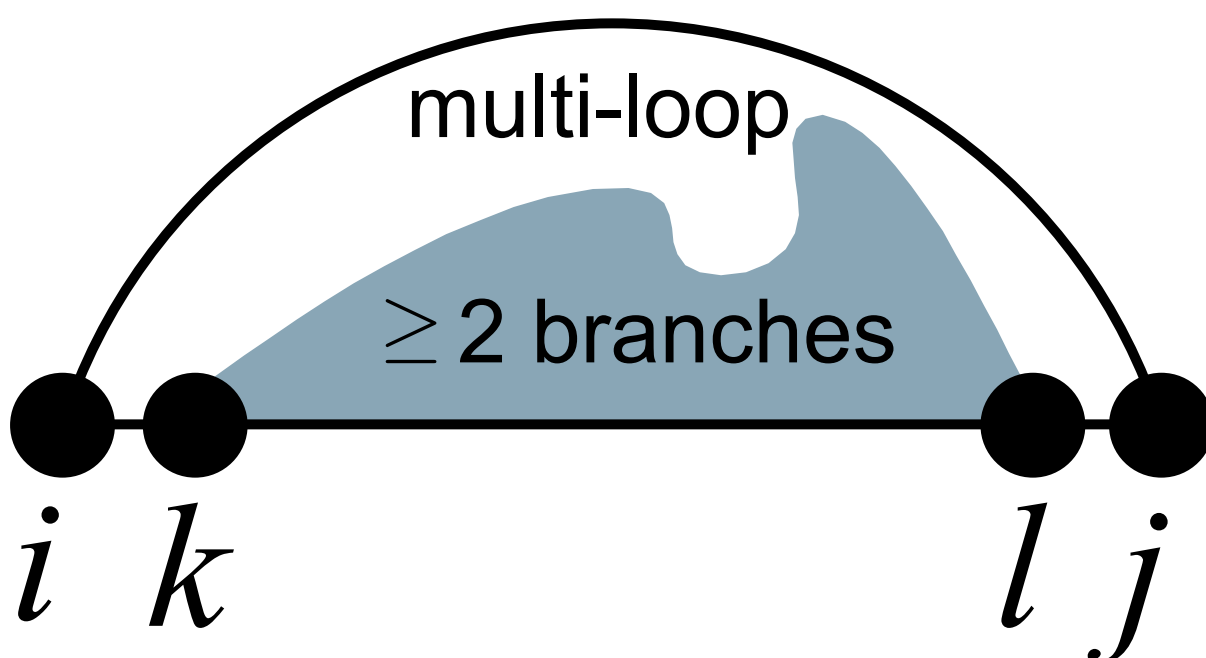


15.9.2.6 `#define VRNA_DECOMP_PAIR_ML 3`

`#include <ViennaRNA/constraints.h>`

Indicator for multibranch loop decomposition step.

This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates a multi-branch loop enclosed by the base pair (i, j) , and consisting of some enclosed multi loop content from k to l .

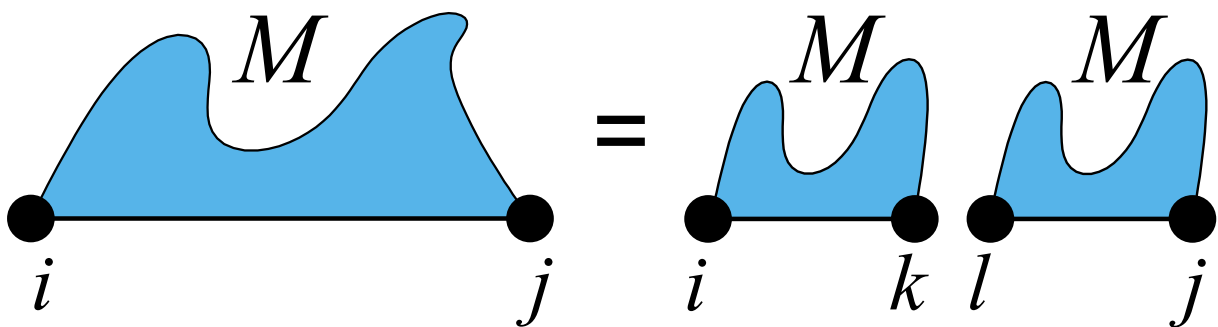


15.9.2.7 `#define VRNA_DECOMP_ML_ML_ML 5`

```
#include <ViennaRNA/constraints.h>
```

Indicator for decomposition of multibranch loop part.

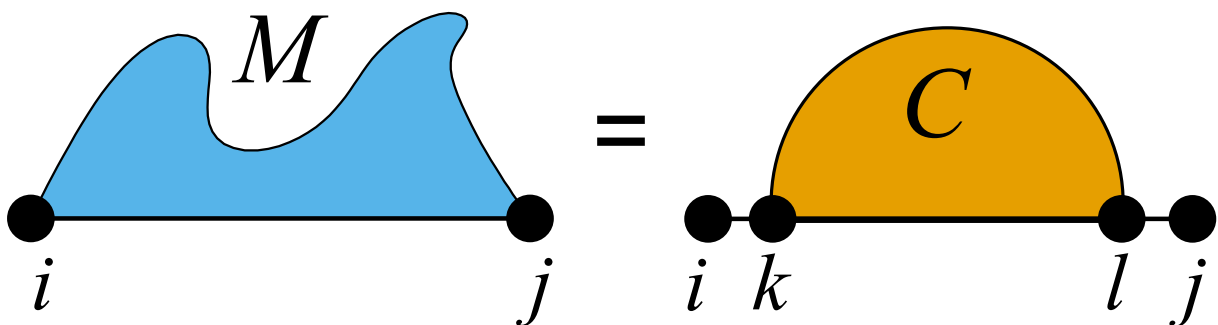
This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates a multi-branch loop part in the interval $[i : j]$, which will be decomposed into two multibranch loop parts $[i : k]$, and $[l : j]$.

15.9.2.8 `#define VRNA_DECOMP_ML_STEM 4`

```
#include <ViennaRNA/constraints.h>
```

Indicator for decomposition of multibranch loop part.

This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates a multi-branch loop part in the interval $[i : j]$, which will be considered a single stem branching off with base pair (k, l) .

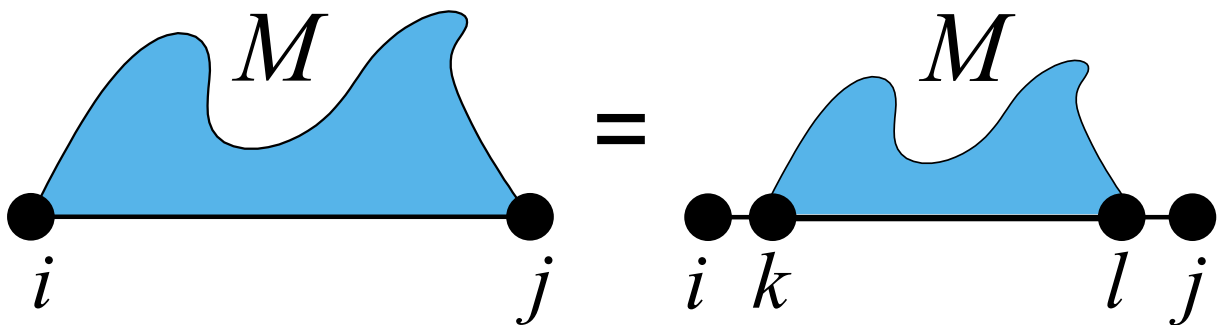


15.9.2.9 #define VRNA_DECOMP_ML_ML 6

```
#include <ViennaRNA/constraints.h>
```

Indicator for decomposition of multibranch loop part.

This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates a multibranch loop part in the interval $[i : j]$, which will be decomposed into a (usually) smaller multibranch loop part $[k : l]$.

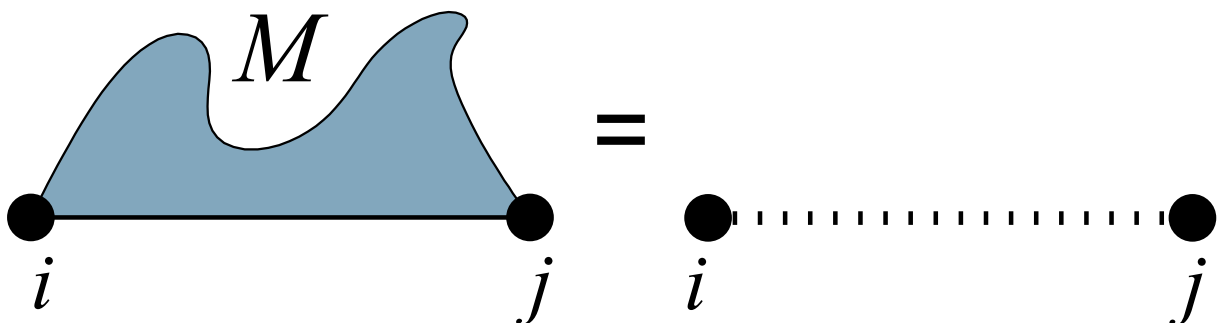


15.9.2.10 #define VRNA_DECOMP_ML_UP 11

```
#include <ViennaRNA/constraints.h>
```

Indicator for decomposition of multibranch loop part.

This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates a multibranch loop part in the interval $[i : j]$, which will be considered a multibranch loop part that only consists of unpaired nucleotides.

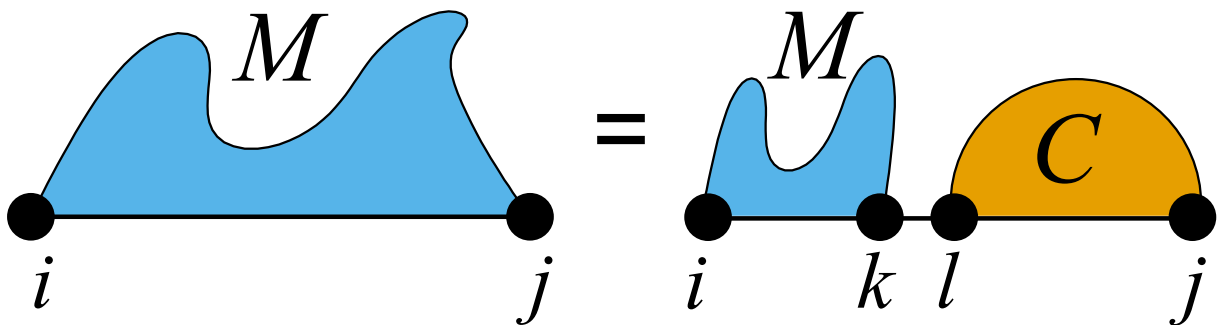


15.9.2.11 `#define VRNA_DECOMP_ML_ML_STEM 20`

```
#include <ViennaRNA/constraints.h>
```

Indicator for decomposition of multibranch loop part.

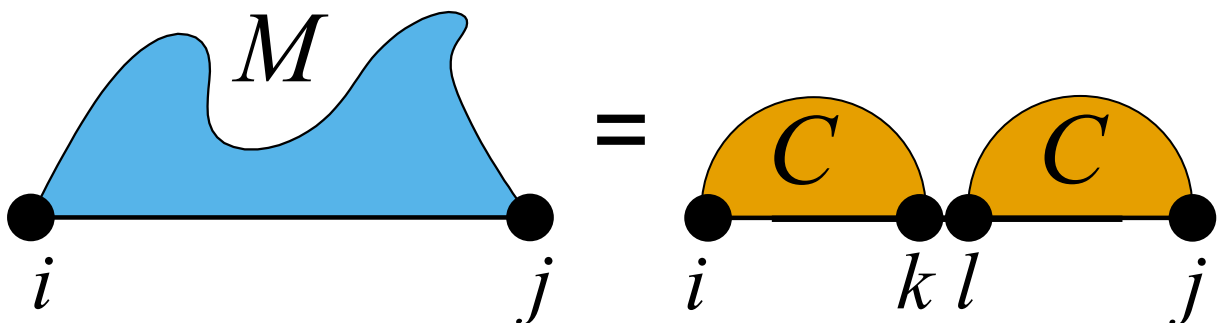
This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates a multibranch loop part in the interval $[i : j]$, which will be decomposed into a multibranch loop part $[i : k]$, and a stem with enclosing base pair (l, j) .

15.9.2.12 `#define VRNA_DECOMP_ML_COAXIAL 13`

```
#include <ViennaRNA/constraints.h>
```

Indicator for decomposition of multibranch loop part.

This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates a multibranch loop part in the interval $[i : j]$, where two stems with enclosing pairs (i, k) and (l, j) are coaxially stacking onto each other.

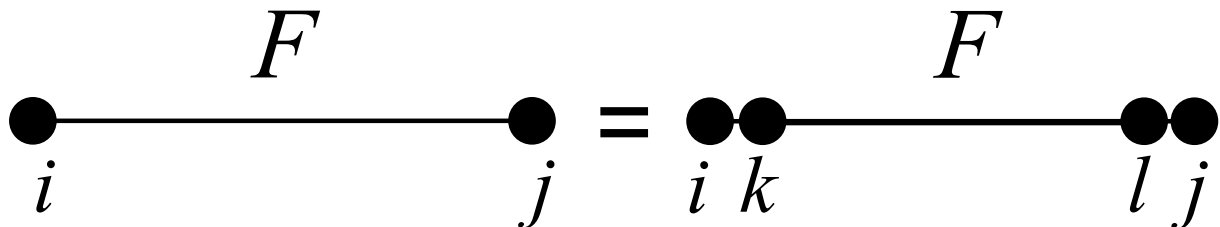


15.9.2.13 `#define VRNA_DECOMP_EXT_EXT 9`

```
#include <ViennaRNA/constraints.h>
```

Indicator for decomposition of exterior loop part.

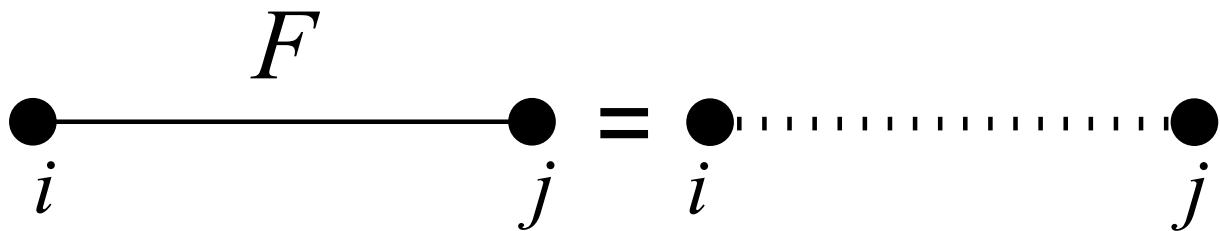
This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates an exterior loop part in the interval $[i : j]$, which will be decomposed into a (usually) smaller exterior loop part $[k : l]$.

15.9.2.14 `#define VRNA_DECOMP_EXT_UP 8`

```
#include <ViennaRNA/constraints.h>
```

Indicator for decomposition of exterior loop part.

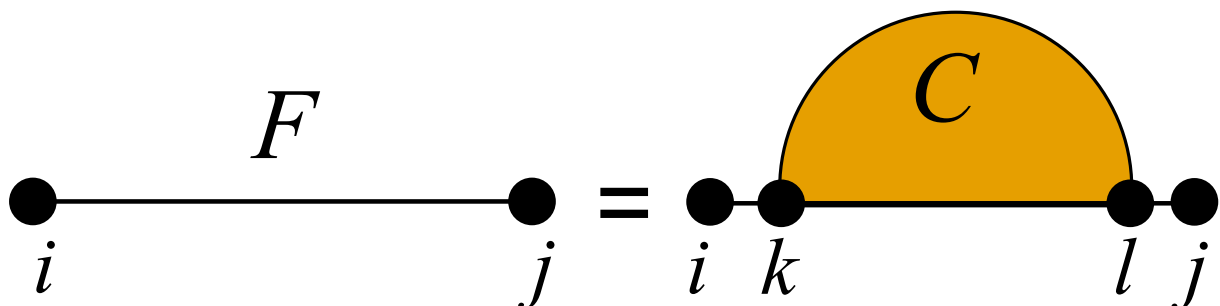
This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates an exterior loop part in the interval $[i : j]$, which will be considered as an exterior loop component consisting of only unpaired nucleotides.

15.9.2.15 `#define VRNA_DECOMP_EXT_STEM 14`

```
#include <ViennaRNA/constraints.h>
```

Indicator for decomposition of exterior loop part.

This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates an exterior loop part in the interval $[i : j]$, which will be considered a stem with enclosing pair (k, l) .

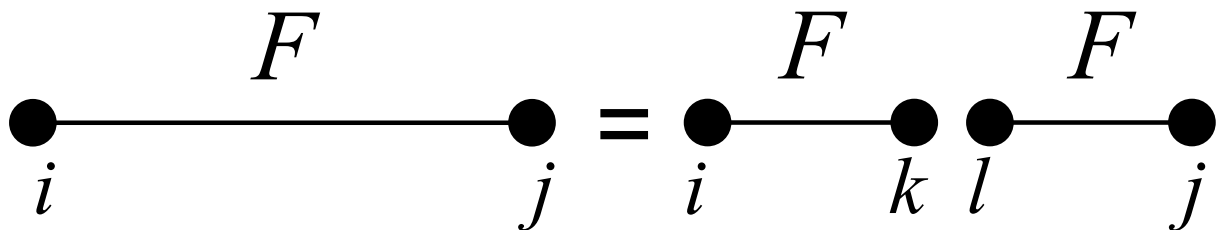


15.9.2.16 `#define VRNA_DECOMP_EXT_EXT_EXT 15`

```
#include <ViennaRNA/constraints.h>
```

Indicator for decomposition of exterior loop part.

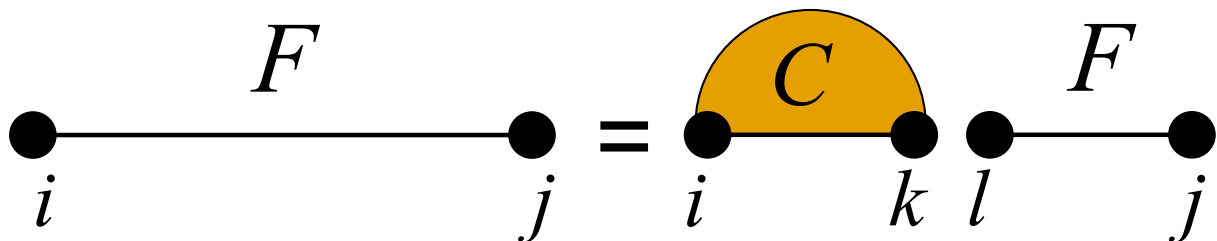
This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates an exterior loop part in the interval $[i : j]$, which will be decomposed into two exterior loop parts $[i : k]$ and $[l : j]$.

15.9.2.17 `#define VRNA_DECOMP_EXT_STEM_EXT 16`

```
#include <ViennaRNA/constraints.h>
```

Indicator for decomposition of exterior loop part.

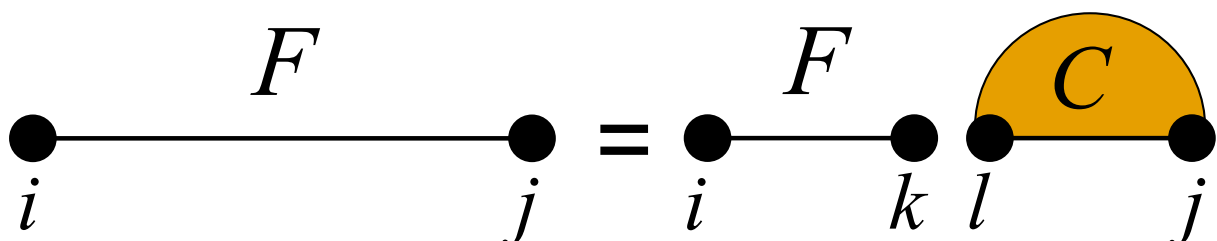
This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates an exterior loop part in the interval $[i : j]$, which will be decomposed into a stem branching off with base pair (i, k) , and an exterior loop part $[l : j]$.

15.9.2.18 `#define VRNA_DECOMP_EXT_EXT_STEM 18`

```
#include <ViennaRNA/constraints.h>
```

Indicator for decomposition of exterior loop part.

This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates an exterior loop part in the interval $[i : j]$, which will be decomposed into an exterior loop part $[i : k]$, and a stem branching off with base pair (l, j) .

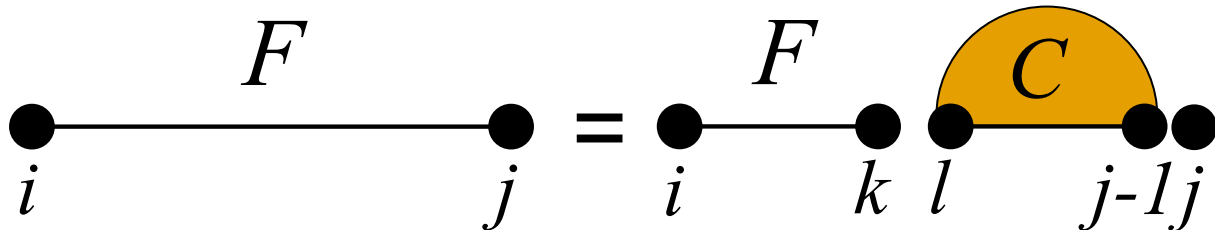


15.9.2.19 #define VRNA_DECOMP_EXT_EXT_STEM1 19

```
#include <ViennaRNA/constraints.h>
```

Indicator for decomposition of exterior loop part.

This flag notifies the soft or hard constraint callback function that the current decomposition step evaluates an exterior loop part in the interval $[i : j]$, which will be decomposed into an exterior loop part $[i : k]$, and a stem branching off with base pair $(l, j - 1)$.



15.9.3 Function Documentation

15.9.3.1 void vrna_constraints_add (vrna_fold_compound_t * vc, const char * constraint, unsigned int options)

```
#include <ViennaRNA/constraints.h>
```

Add constraints to a `vrna_fold_compound_t` data structure.

Use this function to add/update the hard/soft constraints. The function allows for passing a string 'constraint' that can either be a filename that points to a constraints definition file or it may be a pseudo dot-bracket notation indicating hard constraints. For the latter, the user has to pass the `VRNA_CONSTRAINT_DB` option. Also, the user has to specify, which characters are allowed to be interpreted as constraints by passing the corresponding options via the third parameter.

See also

```
vrna_hc_init(), vrna_hc_add_up(), vrna_hc_add_up_batch(), vrna_hc_add_bp(), vrna_sc_init(), vrna_sc_↵
set_up(), vrna_sc_set_bp(), vrna_sc_add_SHAPE_deigan(), vrna_sc_add_SHAPE_zarringhalam(), vrna_↵
_hc_free(), vrna_sc_free(), VRNA_CONSTRAINT_DB, VRNA_CONSTRAINT_DB_DEFAULT, VRNA_CO_↵
NSTRANST_DB_PIPE, VRNA_CONSTRAINT_DB_DOT, VRNA_CONSTRAINT_DB_X, VRNA_CONSTR_↵
INT_DB_ANG_BRACK, VRNA_CONSTRAINT_DB_RND_BRACK, VRNA_CONSTRAINT_DB_INTRAMOL,
VRNA_CONSTRAINT_DB_INTERMOL, VRNA_CONSTRAINT_DB_GQUAD
```

The following is an example for adding hard constraints given in pseudo dot-bracket notation. Here, `vc` is the `vrna_fold_compound_t` object, `structure` is a char array with the hard constraint in dot-bracket notation, and `enforceConstraints` is a flag indicating whether or not constraints for base pairs should be enforced instead of just doing a removal of base pair that conflict with the constraint.

```
unsigned int constraint_options = VRNA_CONSTRAINT_DB_DEFAULT;
if(enforceConstraints)
    constraint_options |= VRNA_CONSTRAINT_DB_ENFORCE_BP;
vrna_constraints_add(vc, (const char *)structure, constraint_options);
```

In contrast to the above, constraints may also be read from file:

```
vrna_constraints_add(vc, constraints_file,
VRNA_OPTION_MFE | ((pf) ? VRNA_OPTION_PF : 0));
```

See also

```
vrna_hc_add_from_db(), vrna_hc_add_up(), vrna_hc_add_up_batch() vrna_hc_add_bp_unspecific(), vrna_↵
_hc_add_bp()
```

Parameters

<i>vc</i>	The fold compound
<i>constraint</i>	A string with either the filename of the constraint definitions or a pseudo dot-bracket notation of the hard constraint. May be NULL.
<i>options</i>	The option flags

15.9.3.2 void vrna_message_constraint_options (unsigned int *option*)

```
#include <ViennaRNA/constraints_hard.h>
```

Print a help message for pseudo dot-bracket structure constraint characters to stdout. (constraint support is specified by option parameter)

Currently available options are:

[VRNA_CONSTRAINT_DB_PIPE](#) (paired with another base)
[VRNA_CONSTRAINT_DB_DOT](#) (no constraint at all)
[VRNA_CONSTRAINT_DB_X](#) (base must not pair)
[VRNA_CONSTRAINT_DB_ANG_BRACK](#) (paired downstream/upstream)
[VRNA_CONSTRAINT_DB_RND_BRACK](#) (base i pairs base j)
 pass a collection of options as one value like this:

```
vrna_message_constraints(option_1 | option_2 | option_n)
```

See also

[vrna_message_constraint_options_all\(\)](#), [vrna_constraints_add\(\)](#), [VRNA_CONSTRAINT_DB](#), [VRNA_CONSTRAINT_DB_PIPE](#), [VRNA_CONSTRAINT_DB_DOT](#), [VRNA_CONSTRAINT_DB_X](#), [VRNA_CONSTRAINT_DB_ANG_BRACK](#), [VRNA_CONSTRAINT_DB_RND_BRACK](#), [VRNA_CONSTRAINT_DB_INTERMOL](#), [VRNA_CONSTRAINT_DB_INTRAMOL](#)

Parameters

<i>option</i>	Option switch that tells which constraint help will be printed
---------------	----------------------------------------------------------------

15.9.3.3 void vrna_message_constraint_options_all (void)

```
#include <ViennaRNA/constraints_hard.h>
```

Print structure constraint characters to stdout (full constraint support)

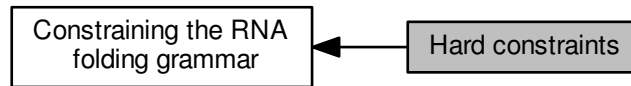
See also

[vrna_message_constraint_options\(\)](#), [vrna_constraints_add\(\)](#), [VRNA_CONSTRAINT_DB](#), [VRNA_CONSTRAINT_DB_PIPE](#), [VRNA_CONSTRAINT_DB_DOT](#), [VRNA_CONSTRAINT_DB_X](#), [VRNA_CONSTRAINT_DB_ANG_BRACK](#), [VRNA_CONSTRAINT_DB_RND_BRACK](#), [VRNA_CONSTRAINT_DB_INTERMOL](#), [VRNA_CONSTRAINT_DB_INTRAMOL](#)

15.10 Hard constraints

This module covers all functionality for hard constraints in secondary structure prediction.

Collaboration diagram for Hard constraints:



Files

- file [constraints_hard.h](#)
Functions and data structures for handling of secondary structure hard constraints.

Data Structures

- struct [vrna_hc_s](#)
The hard constraints data structure. [More...](#)
- struct [vrna_hc_up_s](#)
A single hard constraint for a single nucleotide. [More...](#)

Macros

- `#define VRNA_CONSTRAINT_DB 16384U`
Flag for [vrna_constraints_add\(\)](#) to indicate that constraint is passed in pseudo dot-bracket notation.
- `#define VRNA_CONSTRAINT_DB_ENFORCE_BP 32768U`
Switch for dot-bracket structure constraint to enforce base pairs.
- `#define VRNA_CONSTRAINT_DB_PIPE 65536U`
Flag that is used to indicate the pipe '|' sign in pseudo dot-bracket notation of hard constraints.
- `#define VRNA_CONSTRAINT_DB_DOT 131072U`
dot '.' switch for structure constraints (no constraint at all)
- `#define VRNA_CONSTRAINT_DB_X 262144U`
'x' switch for structure constraint (base must not pair)
- `#define VRNA_CONSTRAINT_DB_RND_BRACK 1048576U`
round brackets '(',')' switch for structure constraint (base i pairs base j)
- `#define VRNA_CONSTRAINT_DB_INTRAMOL 2097152U`
Flag that is used to indicate the character 'I' in pseudo dot-bracket notation of hard constraints.
- `#define VRNA_CONSTRAINT_DB_INTERMOL 4194304U`
Flag that is used to indicate the character 'e' in pseudo dot-bracket notation of hard constraints.
- `#define VRNA_CONSTRAINT_DB_GQUAD 8388608U`
'+' switch for structure constraint (base is involved in a quad)
- `#define VRNA_CONSTRAINT_DB_DEFAULT`

- Switch for dot-bracket structure constraint with default symbols.
- `#define VRNA_CONSTRAINT_CONTEXT_EXT_LOOP (char)0x01`
Hard constraints flag, base pair in the exterior loop.
- `#define VRNA_CONSTRAINT_CONTEXT_HP_LOOP (char)0x02`
Hard constraints flag, base pair encloses hairpin loop.
- `#define VRNA_CONSTRAINT_CONTEXT_INT_LOOP (char)0x04`
Hard constraints flag, base pair encloses an interior loop.
- `#define VRNA_CONSTRAINT_CONTEXT_INT_LOOP_ENC (char)0x08`
Hard constraints flag, base pair encloses a multi branch loop.
- `#define VRNA_CONSTRAINT_CONTEXT_MB_LOOP (char)0x10`
Hard constraints flag, base pair is enclosed in an interior loop.
- `#define VRNA_CONSTRAINT_CONTEXT_MB_LOOP_ENC (char)0x20`
Hard constraints flag, base pair is enclosed in a multi branch loop.
- `#define VRNA_CONSTRAINT_CONTEXT_ALL_LOOPS`
Hard constraints flag, shortcut for all base pairs.

Typedefs

- `typedef struct vrna_hc_s vrna_hc_t`
Typename for the hard constraints data structure `vrna_hc_s`.
- `typedef struct vrna_hc_up_s vrna_hc_up_t`
Typename for the single nucleotide hard constraint data structure `vrna_hc_up_s`.
- `typedef char(vrna_callback_hc_evaluate)(int i, int j, int k, int l, char d, void *data)`
Callback to evaluate whether or not a particular decomposition step is contributing to the solution space.

Functions

- `void vrna_hc_init(vrna_fold_compound_t *vc)`
Initialize/Reset hard constraints to default values.
- `void vrna_hc_add_up(vrna_fold_compound_t *vc, int i, char option)`
Make a certain nucleotide unpaired.
- `int vrna_hc_add_up_batch(vrna_fold_compound_t *vc, vrna_hc_up_t *constraints)`
Apply a list of hard constraints for single nucleotides.
- `void vrna_hc_add_bp(vrna_fold_compound_t *vc, int i, int j, char option)`
Favorize/Enforce a certain base pair (i,j)
- `void vrna_hc_add_bp_nonspecific(vrna_fold_compound_t *vc, int i, int d, char option)`
Enforce a nucleotide to be paired (upstream/downstream)
- `void vrna_hc_free(vrna_hc_t *hc)`
Free the memory allocated by a `vrna_hc_t` data structure.
- `int vrna_hc_add_from_db(vrna_fold_compound_t *vc, const char *constraint, unsigned int options)`
Add hard constraints from pseudo dot-bracket notation.

15.10.1 Detailed Description

This module covers all functionality for hard constraints in secondary structure prediction.

15.10.2 Data Structure Documentation

15.10.2.1 struct vrna_hc_s

The hard constraints data structure.

The content of this data structure determines the decomposition pattern used in the folding recursions. Attribute 'matrix' is used as source for the branching pattern of the decompositions during all folding recursions. Any entry in matrix[i,j] consists of the 6 LSB that allows one to distinguish the following types of base pairs:

- in the exterior loop ([VRNA_CONSTRAINT_CONTEXT_EXT_LOOP](#))
- enclosing a hairpin ([VRNA_CONSTRAINT_CONTEXT_HP_LOOP](#))
- enclosing an interior loop ([VRNA_CONSTRAINT_CONTEXT_INT_LOOP](#))
- enclosed by an exterior loop ([VRNA_CONSTRAINT_CONTEXT_INT_LOOP_ENC](#))
- enclosing a multi branch loop ([VRNA_CONSTRAINT_CONTEXT_MB_LOOP](#))
- enclosed by a multi branch loop ([VRNA_CONSTRAINT_CONTEXT_MB_LOOP_ENC](#))

The four linear arrays 'up_XXX' provide the number of available unpaired nucleotides (including position i) 3' of each position in the sequence.

See also

[vrna_hc_init\(\)](#), [vrna_hc_free\(\)](#), [VRNA_CONSTRAINT_CONTEXT_EXT_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_HP_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_INT_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_MB_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_MB_LOOP_ENC](#)

Data Fields

- char * [matrix](#)
Upper triangular matrix that encodes where a base pair or unpaired nucleotide is allowed.
- int * [up_ext](#)
A linear array that holds the number of allowed unpaired nucleotides in an exterior loop.
- int * [up_hp](#)
A linear array that holds the number of allowed unpaired nucleotides in a hairpin loop.
- int * [up_int](#)
A linear array that holds the number of allowed unpaired nucleotides in an interior loop.
- int * [up_ml](#)
A linear array that holds the number of allowed unpaired nucleotides in a multi branched loop.
- [vrna_callback_hc_evaluate](#) * f
A function pointer that returns whether or not a certain decomposition may be evaluated.
- void * [data](#)
A pointer to some structure where the user may store necessary data to evaluate its generic hard constraint function.
- [vrna_callback_free_auxdata](#) * [free_data](#)
A pointer to a function to free memory occupied by auxiliary data.

15.10.2.1.1 Field Documentation

15.10.2.1.1.1 `vrna_callback_free_auxdata* vrna_hc_s::free_data`

A pointer to a function to free memory occupied by auxiliary data.

The function this pointer is pointing to will be called upon destruction of the `vrna_hc_s`, and provided with the `vrna_hc_s.data` pointer that may hold auxiliary data. Hence, to avoid leaking memory, the user may use this pointer to free memory occupied by auxiliary data.

15.10.2.2 `struct vrna_hc_up_s`

A single hard constraint for a single nucleotide.

Data Fields

- int `position`
The sequence position (1-based)
- char `options`
The hard constraint option.

15.10.3 Macro Definition Documentation

15.10.3.1 `#define VRNA_CONSTRAINT_DB 16384U`

```
#include <ViennaRNA/constraints_hard.h>
```

Flag for `vrna_constraints_add()` to indicate that constraint is passed in pseudo dot-bracket notation.

See also

`vrna_constraints_add()`, `vrna_message_constraint_options()`, `vrna_message_constraint_options_all()`

15.10.3.2 `#define VRNA_CONSTRAINT_DB_ENFORCE_BP 32768U`

```
#include <ViennaRNA/constraints_hard.h>
```

Switch for dot-bracket structure constraint to enforce base pairs.

This flag should be used to really enforce base pairs given in dot-bracket constraint rather than just weakly-enforcing them.

See also

`vrna_hc_add_from_db()`, `vrna_constraints_add()`, `vrna_message_constraint_options()`, `vrna_message_constraint_options_all()`

15.10.3.3 #define VRNA_CONSTRAINT_DB_PIPE 65536U

```
#include <ViennaRNA/constraints_hard.h>
```

Flag that is used to indicate the pipe '|' sign in pseudo dot-bracket notation of hard constraints.

Use this definition to indicate the pipe sign '|' (paired with another base)

See also

[vrna_hc_add_from_db\(\)](#), [vrna_constraints_add\(\)](#), [vrna_message_constraint_options\(\)](#), [vrna_message_constraint_options_all\(\)](#)

15.10.3.4 #define VRNA_CONSTRAINT_DB_DOT 131072U

```
#include <ViennaRNA/constraints_hard.h>
```

dot '.' switch for structure constraints (no constraint at all)

See also

[vrna_hc_add_from_db\(\)](#), [vrna_constraints_add\(\)](#), [vrna_message_constraint_options\(\)](#), [vrna_message_constraint_options_all\(\)](#)

15.10.3.5 #define VRNA_CONSTRAINT_DB_X 262144U

```
#include <ViennaRNA/constraints_hard.h>
```

'x' switch for structure constraint (base must not pair)

See also

[vrna_hc_add_from_db\(\)](#), [vrna_constraints_add\(\)](#), [vrna_message_constraint_options\(\)](#), [vrna_message_constraint_options_all\(\)](#)

15.10.3.6 #define VRNA_CONSTRAINT_DB_RND_BRACK 1048576U

```
#include <ViennaRNA/constraints_hard.h>
```

round brackets '(',')' switch for structure constraint (base i pairs base j)

See also

[vrna_hc_add_from_db\(\)](#), [vrna_constraints_add\(\)](#), [vrna_message_constraint_options\(\)](#), [vrna_message_constraint_options_all\(\)](#)

15.10.3.7 #define VRNA_CONSTRAINT_DB_INTRAMOL 2097152U

```
#include <ViennaRNA/constraints_hard.h>
```

Flag that is used to indicate the character 'l' in pseudo dot-bracket notation of hard constraints.

Use this definition to indicate the usage of 'l' character (intramolecular pairs only)

See also

[vrna_hc_add_from_db\(\)](#), [vrna_constraints_add\(\)](#), [vrna_message_constraint_options\(\)](#), [vrna_message_constraint_options_all\(\)](#)

15.10.3.8 #define VRNA_CONSTRAINT_DB_INTERMOL 4194304U

```
#include <ViennaRNA/constraints_hard.h>
```

Flag that is used to indicate the character 'e' in pseudo dot-bracket notation of hard constraints.

Use this definition to indicate the usage of 'e' character (intermolecular pairs only)

See also

[vrna_hc_add_from_db\(\)](#), [vrna_constraints_add\(\)](#), [vrna_message_constraint_options\(\)](#), [vrna_message_constraint_options_all\(\)](#)

15.10.3.9 #define VRNA_CONSTRAINT_DB_GQUAD 8388608U

```
#include <ViennaRNA/constraints_hard.h>
```

'+' switch for structure constraint (base is involved in a quad)

See also

[vrna_hc_add_from_db\(\)](#), [vrna_constraints_add\(\)](#), [vrna_message_constraint_options\(\)](#), [vrna_message_constraint_options_all\(\)](#)

Warning

This flag is for future purposes only! No implementation recognizes it yet.

15.10.3.10 #define VRNA_CONSTRAINT_DB_DEFAULT

```
#include <ViennaRNA/constraints_hard.h>
```

Value:

```
(
    VRNA_CONSTRAINT_DB \
    | VRNA_CONSTRAINT_DB_PIPE \
    | VRNA_CONSTRAINT_DB_DOT \
    | VRNA_CONSTRAINT_DB_X \
    | VRNA_CONSTRAINT_DB_ANG_BRACK \
    | VRNA_CONSTRAINT_DB_RND_BRACK \
    | VRNA_CONSTRAINT_DB_INTRAMOL \
    | VRNA_CONSTRAINT_DB_INTERMOL \
    | VRNA_CONSTRAINT_DB_GQUAD \
)
```

Switch for dot-bracket structure constraint with default symbols.

This flag conveniently combines all possible symbols in dot-bracket notation for hard constraints and [VRNA_CONSTRAINT_DB](#)

See also

[vrna_hc_add_from_db\(\)](#), [vrna_constraints_add\(\)](#), [vrna_message_constraint_options\(\)](#), [vrna_message_constraint_options_all\(\)](#)

15.10.4 Typedef Documentation

15.10.4.1 typedef char(vrna_callback_hc_evaluate)(int i, int j, int k, int l, char d, void *data)

```
#include <ViennaRNA/constraints_hard.h>
```

Callback to evaluate whether or not a particular decomposition step is contributing to the solution space.

This is the prototype for callback functions used by the folding recursions to evaluate generic hard constraints. The first four parameters passed indicate the delimiting nucleotide positions of the decomposition, and the parameter `denotes` the decomposition step. The last parameter `data` is the auxiliary data structure associated to the hard constraints via `vrna_hc_add_data()`, or NULL if no auxiliary data was added.

See also

[VRNA_DECOMP_PAIR_HP](#), [VRNA_DECOMP_PAIR_IL](#), [VRNA_DECOMP_PAIR_ML](#), [VRNA_DECOMP_ML_ML_ML](#), [VRNA_DECOMP_ML_STEM](#), [VRNA_DECOMP_ML_ML](#), [VRNA_DECOMP_ML_UP](#), [VRNA_DECOMP_ML_ML_STEM](#), [VRNA_DECOMP_ML_COAXIAL](#), [VRNA_DECOMP_EXT_EXT](#), [VRNA_DECOMP_EXT_UP](#), [VRNA_DECOMP_EXT_STEM](#), [VRNA_DECOMP_EXT_EXT_EXT](#), [VRNA_DECOMP_EXT_STEM_EXT](#), [VRNA_DECOMP_EXT_EXT_STEM](#), [VRNA_DECOMP_EXT_EXT_STEM1](#), [vrna_hc_add_f\(\)](#), [vrna_hc_add_data\(\)](#)

Parameters

<i>i</i>	Left (5') delimiter position of substructure
<i>j</i>	Right (3') delimiter position of substructure
<i>k</i>	Left delimiter of decomposition
<i>l</i>	Right delimiter of decomposition
<i>d</i>	Decomposition step indicator
Generated by Auxiliary data	

Returns

Pseudo energy contribution in deka-kalories per mol

15.10.5 Function Documentation

15.10.5.1 void vrna_hc_init (vrna_fold_compound_t * vc)

```
#include <ViennaRNA/constraints_hard.h>
```

Initialize/Reset hard constraints to default values.

This function resets the hard constraints to their default values, i.e. all positions may be unpaired in all contexts, and base pairs are allowed in all contexts, if they resemble canonical pairs. Previously set hard constraints will be removed before initialization.

See also

[vrna_hc_add_bp\(\)](#), [vrna_hc_add_bp_nonspecific\(\)](#), [vrna_hc_add_up\(\)](#)

Parameters

vc	The fold compound
----	-------------------

SWIG Wrapper Notes This function is attached as method **hc_init()** to objects of type *fold_compound*

15.10.5.2 void vrna_hc_add_up (vrna_fold_compound_t * vc, int i, char option)

```
#include <ViennaRNA/constraints_hard.h>
```

Make a certain nucleotide unpaired.

See also

[vrna_hc_add_bp\(\)](#), [vrna_hc_add_bp_nonspecific\(\)](#), [vrna_hc_init\(\)](#), [VRNA_CONSTRAINT_CONTEXT_EX→XT_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_HP_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_INT_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_MB_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_ALL_LOOPS](#)

Parameters

vc	The vrna_fold_compound_t the hard constraints are associated with
i	The position that needs to stay unpaired (1-based)
option	The options flag indicating how/where to store the hard constraints

SWIG Wrapper Notes This function is attached as method **hc_add_up()** to objects of type *fold_compound*

15.10.5.3 `int vrna_hc_add_up_batch (vrna_fold_compound_t * vc, vrna_hc_up_t * constraints)`

```
#include <ViennaRNA/constraints_hard.h>
```

Apply a list of hard constraints for single nucleotides.

Parameters

<code>vc</code>	The vrna_fold_compound_t the hard constraints are associated with
<code>constraints</code>	The list of constraints to apply, last entry must have position attribute set to 0

15.10.5.4 `void vrna_hc_add_bp (vrna_fold_compound_t * vc, int i, int j, char option)`

```
#include <ViennaRNA/constraints_hard.h>
```

Favorize/Enforce a certain base pair (i,j)

See also

[vrna_hc_add_bp_nonspecific\(\)](#), [vrna_hc_add_up\(\)](#), [vrna_hc_init\(\)](#), [VRNA_CONSTRAINT_CONTEXT_EXT_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_HP_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_INT_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_INT_LOOP_ENC](#), [VRNA_CONSTRAINT_CONTEXT_MB_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_MB_LOOP_ENC](#), [VRNA_CONSTRAINT_CONTEXT_ENFORCE](#), [VRNA_CONSTRAINT_CONTEXT_ALL_LOOPS](#)

Parameters

<code>vc</code>	The vrna_fold_compound_t the hard constraints are associated with
<code>i</code>	The 5' located nucleotide position of the base pair (1-based)
<code>j</code>	The 3' located nucleotide position of the base pair (1-based)
<code>option</code>	The options flag indicating how/where to store the hard constraints

SWIG Wrapper Notes This function is attached as method **hc_add_bp()** to objects of type *fold_compound*

15.10.5.5 `void vrna_hc_add_bp_nonspecific (vrna_fold_compound_t * vc, int i, int d, char option)`

```
#include <ViennaRNA/constraints_hard.h>
```

Enforce a nucleotide to be paired (upstream/downstream)

See also

[vrna_hc_add_bp\(\)](#), [vrna_hc_add_up\(\)](#), [vrna_hc_init\(\)](#), [VRNA_CONSTRAINT_CONTEXT_EXT_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_HP_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_INT_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_INT_LOOP_ENC](#), [VRNA_CONSTRAINT_CONTEXT_MB_LOOP](#), [VRNA_CONSTRAINT_CONTEXT_MB_LOOP_ENC](#), [VRNA_CONSTRAINT_CONTEXT_ENFORCE](#), [VRNA_CONSTRAINT_CONTEXT_ALL_LOOPS](#)

Parameters

<i>vc</i>	The vrna_fold_compound_t the hard constraints are associated with
<i>i</i>	The position that needs to stay unpaired (1-based)
<i>d</i>	The direction of base pairing ($d < 0$: pairs upstream, $d > 0$: pairs downstream, $d == 0$: no direction)
<i>option</i>	The options flag indicating in which loop type context the pairs may appear

SWIG Wrapper Notes This function is attached as method **hc_add_bp_nonspecific()** to objects of type *fold_compound*

15.10.5.6 void vrna_hc_free (vrna_hc_t * hc)

```
#include <ViennaRNA/constraints_hard.h>
```

Free the memory allocated by a [vrna_hc_t](#) data structure.

Use this function to free all memory that was allocated for a data structure of type [vrna_hc_t](#).

See also

[get_hard_constraints\(\)](#), [vrna_hc_t](#)

15.10.5.7 int vrna_hc_add_from_db (vrna_fold_compound_t * vc, const char * constraint, unsigned int options)

```
#include <ViennaRNA/constraints_hard.h>
```

Add hard constraints from pseudo dot-bracket notation.

This function allows one to apply hard constraints from a pseudo dot-bracket notation. The `options` parameter controls, which characters are recognized by the parser. Use the [VRNA_CONSTRAINT_DB_DEFAULT](#) convenience macro, if you want to allow all known characters

See also

[VRNA_CONSTRAINT_DB_PIPE](#), [VRNA_CONSTRAINT_DB_DOT](#), [VRNA_CONSTRAINT_DB_X](#), [VRNA_CONSTRAINT_DB_ANG_BRACK](#), [VRNA_CONSTRAINT_DB_RND_BRACK](#), [VRNA_CONSTRAINT_DB_INTRAMOL](#), [VRNA_CONSTRAINT_DB_INTERMOL](#), [VRNA_CONSTRAINT_DB_GQUAD](#)

Parameters

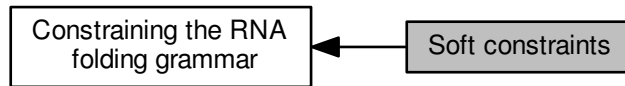
<i>vc</i>	The fold compound
<i>constraint</i>	A pseudo dot-bracket notation of the hard constraint.
<i>options</i>	The option flags

SWIG Wrapper Notes This function is attached as method **hc_add_from_db()** to objects of type *fold_compound*

15.11 Soft constraints

Functions and data structures for secondary structure soft constraints.

Collaboration diagram for Soft constraints:



Files

- file [constraints_soft.h](#)
Functions and data structures for secondary structure soft constraints.

Data Structures

- struct [vrna_sc_s](#)
The soft constraints data structure. [More...](#)

Typedefs

- typedef struct [vrna_sc_s](#) [vrna_sc_t](#)
Typename for the soft constraints data structure [vrna_sc_s](#).
- typedef int([vrna_callback_sc_energy](#)) (int i, int j, int k, int l, char d, void *data)
Callback to retrieve pseudo energy contribution for soft constraint feature.
- typedef [FLT_OR_DBL](#)([vrna_callback_sc_exp_energy](#)) (int i, int j, int k, int l, char d, void *data)
Callback to retrieve pseudo energy contribution as Boltzmann Factors for soft constraint feature.
- typedef [vrna_basepair_t](#) *([vrna_callback_sc_backtrack](#)) (int i, int j, int k, int l, char d, void *data)
Callback to retrieve auxiliary base pairs for soft constraint feature.

Functions

- void [vrna_sc_init](#) ([vrna_fold_compound_t](#) *vc)
Initialize an empty soft constraints data structure within a [vrna_fold_compound_t](#).
- void [vrna_sc_set_bp](#) ([vrna_fold_compound_t](#) *vc, const [FLT_OR_DBL](#) **constraints, unsigned int options)
Set soft constraints for paired nucleotides.
- void [vrna_sc_add_bp](#) ([vrna_fold_compound_t](#) *vc, int i, int j, [FLT_OR_DBL](#) energy, unsigned int options)
Add soft constraints for paired nucleotides.
- void [vrna_sc_set_up](#) ([vrna_fold_compound_t](#) *vc, const [FLT_OR_DBL](#) *constraints, unsigned int options)
Set soft constraints for unpaired nucleotides.
- void [vrna_sc_add_up](#) ([vrna_fold_compound_t](#) *vc, int i, [FLT_OR_DBL](#) energy, unsigned int options)

- *Add soft constraints for unpaired nucleotides.*
- void `vrna_sc_remove` (`vrna_fold_compound_t` *vc)
- *Remove soft constraints from `vrna_fold_compound_t`.*
- void `vrna_sc_free` (`vrna_sc_t` *sc)
- *Free memory occupied by a `vrna_sc_t` data structure.*
- void `vrna_sc_add_data` (`vrna_fold_compound_t` *vc, void *data, `vrna_callback_free_auxdata` *free_data)
- *Add an auxiliary data structure for the generic soft constraints callback function.*
- void `vrna_sc_add_f` (`vrna_fold_compound_t` *vc, `vrna_callback_sc_energy` *f)
- *Bind a function pointer for generic soft constraint feature (MFE version)*
- void `vrna_sc_add_bt` (`vrna_fold_compound_t` *vc, `vrna_callback_sc_backtrack` *f)
- *Bind a backtracking function pointer for generic soft constraint feature.*
- void `vrna_sc_add_exp_f` (`vrna_fold_compound_t` *vc, `vrna_callback_sc_exp_energy` *exp_f)
- *Bind a function pointer for generic soft constraint feature (PF version)*

15.11.1 Detailed Description

Functions and data structures for secondary structure soft constraints.

Soft-constraints are used to change position specific contributions in the recursions by adding bonuses/penalties in form of pseudo free energies to certain loop configurations.

15.11.2 Data Structure Documentation

15.11.2.1 struct `vrna_sc_s`

The soft constraints data structure.

Data Fields

- int ** `energy_up`
- *Energy contribution for stretches of unpaired nucleotides.*
- int * `energy_bp`
- *Energy contribution for base pairs.*
- FLT_OR_DBL ** `exp_energy_up`
- *Boltzmann Factors of the energy contributions for unpaired sequence stretches.*
- FLT_OR_DBL * `exp_energy_bp`
- *Boltzmann Factors of the energy contribution for base pairs.*
- int * `energy_stack`
- *Pseudo Energy contribution per base pair involved in a stack.*
- FLT_OR_DBL * `exp_energy_stack`
- *Boltzmann weighted pseudo energy contribution per nucleotide involved in a stack.*
- `vrna_callback_sc_energy` * f
- *A function pointer used for pseudo energy contribution in MFE calculations.*
- `vrna_callback_sc_backtrack` * bt
- *A function pointer used to obtain backtraced base pairs in loop regions that were altered by soft constrained pseudo energy contributions.*
- `vrna_callback_sc_exp_energy` * exp_f
- *A function pointer used for pseudo energy contribution boltzmann factors in PF calculations.*
- void * `data`
- *A pointer to the data object provided for for pseudo energy contribution functions of the generic soft constraints feature.*

15.11.2.1.1 Field Documentation

15.11.2.1.1.1 `vrna_callback_sc_energy* vrna_sc_s::f`

A function pointer used for pseudo energy contribution in MFE calculations.

See also

[vrna_sc_add_f\(\)](#)

15.11.2.1.1.2 `vrna_callback_sc_backtrack* vrna_sc_s::bt`

A function pointer used to obtain backtraced base pairs in loop regions that were altered by soft constrained pseudo energy contributions.

See also

[vrna_sc_add_bt\(\)](#)

15.11.2.1.1.3 `vrna_callback_sc_exp_energy* vrna_sc_s::exp_f`

A function pointer used for pseudo energy contribution boltzmann factors in PF calculations.

See also

[vrna_sc_add_exp_f\(\)](#)

15.11.3 Typedef Documentation

15.11.3.1 `typedef int(vrna_callback_sc_energy) (int i, int j, int k, int l, char d, void *data)`

```
#include <ViennaRNA/constraints_soft.h>
```

Callback to retrieve pseudo energy contribution for soft constraint feature.

This is the prototype for callback functions used by the folding recursions to evaluate generic soft constraints. The first four parameters passed indicate the delimiting nucleotide positions of the decomposition, and the parameter `denotes` the decomposition step. The last parameter `data` is the auxiliary data structure associated to the hard constraints via [vrna_sc_add_data\(\)](#), or NULL if no auxiliary data was added.

See also

[VRNA_DECOMP_PAIR_HP](#), [VRNA_DECOMP_PAIR_IL](#), [VRNA_DECOMP_PAIR_ML](#), [VRNA_DECOMP_ML_ML_ML](#), [VRNA_DECOMP_ML_STEM](#), [VRNA_DECOMP_ML_ML](#), [VRNA_DECOMP_ML_UP](#), [VRNA_DECOMP_ML_ML_STEM](#), [VRNA_DECOMP_ML_COAXIAL](#), [VRNA_DECOMP_EXT_EXT](#), [VRNA_DECOMP_EXT_UP](#), [VRNA_DECOMP_EXT_STEM](#), [VRNA_DECOMP_EXT_EXT_EXT](#), [VRNA_DECOMP_EXT_STEM_EXT](#), [VRNA_DECOMP_EXT_EXT_STEM](#), [VRNA_DECOMP_EXT_EXT_STEM1](#), [vrna_sc_add_f\(\)](#), [vrna_sc_add_exp_f\(\)](#), [vrna_sc_add_bt\(\)](#), [vrna_sc_add_data\(\)](#)

Parameters

<i>i</i>	Left (5') delimiter position of substructure
<i>j</i>	Right (3') delimiter position of substructure
<i>k</i>	Left delimiter of decomposition
<i>l</i>	Right delimiter of decomposition
<i>d</i>	Decomposition step indicator
<i>data</i>	Auxiliary data

Returns

Pseudo energy contribution in deka-kalories per mol

15.11.3.2 `typedef FLT_OR_DBL(vrna_callback_sc_exp_energy)(int i, int j, int k, int l, char d, void *data)`

```
#include <ViennaRNA/constraints_soft.h>
```

Callback to retrieve pseudo energy contribution as Boltzmann Factors for soft constraint feature.

This is the prototype for callback functions used by the partition function recursions to evaluate generic soft constraints. The first four parameters passed indicate the delimiting nucleotide positions of the decomposition, and the parameter `denotes` the decomposition step. The last parameter `data` is the auxiliary data structure associated to the hard constraints via `vrna_sc_add_data()`, or NULL if no auxiliary data was added.

See also

[VRNA_DECOMP_PAIR_HP](#), [VRNA_DECOMP_PAIR_IL](#), [VRNA_DECOMP_PAIR_ML](#), [VRNA_DECOMP_ML_ML_ML](#), [VRNA_DECOMP_ML_STEM](#), [VRNA_DECOMP_ML_ML](#), [VRNA_DECOMP_ML_UP](#), [VRNA_DECOMP_ML_ML_STEM](#), [VRNA_DECOMP_ML_COAXIAL](#), [VRNA_DECOMP_EXT_EXT](#), [VRNA_DECOMP_EXT_UP](#), [VRNA_DECOMP_EXT_STEM](#), [VRNA_DECOMP_EXT_EXT_EXT](#), [VRNA_DECOMP_EXT_STEM_EXT](#), [VRNA_DECOMP_EXT_EXT_STEM](#), [VRNA_DECOMP_EXT_EXT_STEM1](#), [vrna_sc_add_exp_f\(\)](#), [vrna_sc_add_f\(\)](#), [vrna_sc_add_bt\(\)](#), [vrna_sc_add_data\(\)](#)

Parameters

<i>i</i>	Left (5') delimiter position of substructure
<i>j</i>	Right (3') delimiter position of substructure
<i>k</i>	Left delimiter of decomposition
<i>l</i>	Right delimiter of decomposition
<i>d</i>	Decomposition step indicator
<i>data</i>	Auxiliary data

Returns

Pseudo energy contribution in deka-kalories per mol

15.11.3.3 `typedef vrna_basepair_t*(vrna_callback_sc_backtrack)(int i, int j, int k, int l, char d, void *data)`

```
#include <ViennaRNA/constraints_soft.h>
```


Callback to retrieve auxiliary base pairs for soft constraint feature.

See also

[VRNA_DECOMP_PAIR_HP](#), [VRNA_DECOMP_PAIR_IL](#), [VRNA_DECOMP_PAIR_ML](#), [VRNA_DECOMP_ML_ML_ML](#), [VRNA_DECOMP_ML_STEM](#), [VRNA_DECOMP_ML_ML](#), [VRNA_DECOMP_ML_UP](#), [VRNA_DECOMP_ML_ML_STEM](#), [VRNA_DECOMP_ML_COAXIAL](#), [VRNA_DECOMP_EXT_EXT](#), [VRNA_DECOMP_EXT_UP](#), [VRNA_DECOMP_EXT_STEM](#), [VRNA_DECOMP_EXT_EXT_EXT](#), [VRNA_DECOMP_EXT_STEM_EXT](#), [VRNA_DECOMP_EXT_EXT_STEM](#), [VRNA_DECOMP_EXT_EXT_STEM1](#), [vrna_sc_add_bt\(\)](#), [vrna_sc_add_f\(\)](#), [vrna_sc_add_exp_f\(\)](#), [vrna_sc_add_data\(\)](#)

Parameters

<i>i</i>	Left (5') delimiter position of substructure
<i>j</i>	Right (3') delimiter position of substructure
<i>k</i>	Left delimiter of decomposition
<i>l</i>	Right delimiter of decomposition
<i>d</i>	Decomposition step indicator
<i>data</i>	Auxiliary data

Returns

List of additional base pairs

15.11.4 Function Documentation

15.11.4.1 void vrna_sc_init (vrna_fold_compound_t * vc)

```
#include <ViennaRNA/constraints_soft.h>
```

Initialize an empty soft constraints data structure within a [vrna_fold_compound_t](#).

This function adds a proper soft constraints data structure to the [vrna_fold_compound_t](#) data structure. If soft constraints already exist within the fold compound, they are removed.

Note

Accepts [vrna_fold_compound_t](#) of type [VRNA_FC_TYPE_SINGLE](#) and [VRNA_FC_TYPE_COMPARATIVE](#)

See also

[vrna_sc_set_bp\(\)](#), [vrna_sc_set_up\(\)](#), [vrna_sc_add_SHAPE_deigan\(\)](#), [vrna_sc_add_SHAPE_zarringham\(\)](#), [vrna_sc_remove\(\)](#), [vrna_sc_add_f\(\)](#), [vrna_sc_add_exp_f\(\)](#), [vrna_sc_add_pre\(\)](#), [vrna_sc_add_post\(\)](#)

Parameters

<i>vc</i>	The vrna_fold_compound_t where an empty soft constraint feature is to be added to
-----------	---------------------------------------------------------------------------------------------------

SWIG Wrapper Notes This function is attached as method **sc_init()** to objects of type *fold_compound*

15.11.4.2 `void vrna_sc_set_bp (vrna_fold_compound_t * vc, const FLT_OR_DBL ** constraints, unsigned int options)`

```
#include <ViennaRNA/constraints_soft.h>
```

Set soft constraints for paired nucleotides.

Note

This function replaces any pre-existing soft constraints with the ones supplied in `constraints`.

See also

[vrna_sc_add_bp\(\)](#), [vrna_sc_set_up\(\)](#), [vrna_sc_add_up\(\)](#)

Parameters

<i>vc</i>	The vrna_fold_compound_t the soft constraints are associated with
<i>constraints</i>	A two-dimensional array of pseudo free energies in <i>kcal/mol</i>
<i>options</i>	The options flag indicating how/where to store the soft constraints

SWIG Wrapper Notes This function is attached as method `sc_set_bp()` to objects of type *fold_compound*

15.11.4.3 `void vrna_sc_add_bp (vrna_fold_compound_t * vc, int i, int j, FLT_OR_DBL energy, unsigned int options)`

```
#include <ViennaRNA/constraints_soft.h>
```

Add soft constraints for paired nucleotides.

See also

[vrna_sc_set_bp\(\)](#), [vrna_sc_set_up\(\)](#), [vrna_sc_add_up\(\)](#)

Parameters

<i>vc</i>	The vrna_fold_compound_t the soft constraints are associated with
<i>i</i>	The 5' position of the base pair the soft constraint is added for
<i>j</i>	The 3' position of the base pair the soft constraint is added for
<i>energy</i>	The free energy (soft-constraint) in <i>kcal/mol</i>
<i>options</i>	The options flag indicating how/where to store the soft constraints

SWIG Wrapper Notes This function is attached as an overloaded method `sc_add_bp()` to objects of type *fold_compound*. The method either takes arguments for a single base pair (i,j) with the corresponding energy value:

```
00001 fold_compound.sc_add_bp(i, j, energy, options)
```

or an entire 2-dimensional matrix with dimensions $n \times n$ that stores free energy contributions for any base pair (i,j) with $1 \leq i < j \leq n$:

```
00001 fold_compound.sc_add_bp(matrix, options)
```

In both variants, the `options` argument is optional and may be omitted.

15.11.4.4 `void vrna_sc_set_up(vrna_fold_compound_t * vc, const FLT_OR_DBL * constraints, unsigned int options)`

```
#include <ViennaRNA/constraints_soft.h>
```

Set soft constraints for unpaired nucleotides.

Note

This function replaces any pre-existing soft constraints with the ones supplied in `constraints`.

See also

[vrna_sc_add_up\(\)](#), [vrna_sc_set_bp\(\)](#), [vrna_sc_add_bp\(\)](#)

Parameters

<code>vc</code>	The vrna_fold_compound_t the soft constraints are associated with
<code>constraints</code>	A vector of pseudo free energies in <i>kcal/mol</i>
<code>options</code>	The options flag indicating how/where to store the soft constraints

SWIG Wrapper Notes This function is attached as method `sc_set_up()` to objects of type `fold_compound`

15.11.4.5 `void vrna_sc_add_up(vrna_fold_compound_t * vc, int i, FLT_OR_DBL energy, unsigned int options)`

```
#include <ViennaRNA/constraints_soft.h>
```

Add soft constraints for unpaired nucleotides.

See also

[vrna_sc_set_up\(\)](#), [vrna_sc_add_bp\(\)](#), [vrna_sc_set_bp\(\)](#)

Parameters

<code>vc</code>	The vrna_fold_compound_t the soft constraints are associated with
<code>i</code>	The nucleotide position the soft constraint is added for
<code>energy</code>	The free energy (soft-constraint) in <i>kcal/mol</i>
<code>options</code>	The options flag indicating how/where to store the soft constraints

SWIG Wrapper Notes This function is attached as an overloaded method **sc_add_up()** to objects of type *fold_compound*. The method either takes arguments for a single nucleotide i with the corresponding energy value:

```
00001 fold_compound.sc_add_up(i, energy, options)
```

or an entire vector that stores free energy contributions for each nucleotide i with $1 \leq i \leq n$:

```
00001 fold_compound.sc_add_bp(vector, options)
```

In both variants, the `options` argument is optional and can be omitted.

15.11.4.6 `void vrna_sc_remove (vrna_fold_compound_t * vc)`

```
#include <ViennaRNA/constraints_soft.h>
```

Remove soft constraints from `vrna_fold_compound_t`.

Note

Accepts `vrna_fold_compound_t` of type `VRNA_FC_TYPE_SINGLE` and `VRNA_FC_TYPE_COMPARATIVE`

Parameters

<code>vc</code>	The <code>vrna_fold_compound_t</code> possibly containing soft constraints
-----------------	----------------------------------------------------------------------------

SWIG Wrapper Notes This function is attached as method **sc_remove()** to objects of type *fold_compound*

15.11.4.7 `void vrna_sc_free (vrna_sc_t * sc)`

```
#include <ViennaRNA/constraints_soft.h>
```

Free memory occupied by a `vrna_sc_t` data structure.

Parameters

<code>sc</code>	The data structure to free from memory
-----------------	----------------------------------------

15.11.4.8 `void vrna_sc_add_data (vrna_fold_compound_t * vc, void * data, vrna_callback_free_auxdata * free_data)`

```
#include <ViennaRNA/constraints_soft.h>
```

Add an auxiliary data structure for the generic soft constraints callback function.

See also

[vrna_sc_add_f\(\)](#), [vrna_sc_add_exp_f\(\)](#), [vrna_sc_add_bt\(\)](#)

Parameters

<i>vc</i>	The fold compound the generic soft constraint function should be bound to
<i>data</i>	A pointer to the data structure that holds required data for function 'f'
<i>free_data</i>	A pointer to a function that free's the memory occupied by <i>data</i> (Maybe NULL)

SWIG Wrapper Notes This function is attached as method **sc_add_data()** to objects of type *fold_compound*

15.11.4.9 void vrna_sc_add_f(vrna_fold_compound_t * vc, vrna_callback_sc_energy * f)

```
#include <ViennaRNA/constraints_soft.h>
```

Bind a function pointer for generic soft constraint feature (MFE version)

This function allows one to easily bind a function pointer and corresponding data structure to the soft constraint part [vrna_sc_t](#) of the [vrna_fold_compound_t](#). The function for evaluating the generic soft constraint feature has to return a pseudo free energy \hat{E} in *dacal/mol*, where $1\text{dacal/mol} = 10\text{cal/mol}$.

See also

[vrna_sc_add_data\(\)](#), [vrna_sc_add_bt\(\)](#), [vrna_sc_add_exp_f\(\)](#)

Parameters

<i>vc</i>	The fold compound the generic soft constraint function should be bound to
<i>f</i>	A pointer to the function that evaluates the generic soft constraint feature

SWIG Wrapper Notes This function is attached as method **sc_add_f()** to objects of type *fold_compound*

15.11.4.10 void vrna_sc_add_bt(vrna_fold_compound_t * vc, vrna_callback_sc_backtrack * f)

```
#include <ViennaRNA/constraints_soft.h>
```

Bind a backtracking function pointer for generic soft constraint feature.

This function allows one to easily bind a function pointer to the soft constraint part [vrna_sc_t](#) of the [vrna_fold_compound_t](#). The provided function should be used for backtracking purposes in loop regions that were altered via the generic soft constraint feature. It has to return an array of [vrna_basepair_t](#) data structures, where the last element in the list is indicated by a value of -1 in it's *i* position.

See also

[vrna_sc_add_data\(\)](#), [vrna_sc_add_f\(\)](#), [vrna_sc_add_exp_f\(\)](#)

Parameters

<i>vc</i>	The fold compound the generic soft constraint function should be bound to
<i>f</i>	A pointer to the function that returns additional base pairs

SWIG Wrapper Notes This function is attached as method **sc_add_bt()** to objects of type *fold_compound*

15.11.4.11 void vrna_sc_add_exp_f (vrna_fold_compound_t * vc, vrna_callback_sc_exp_energy * exp_f)

```
#include <ViennaRNA/constraints_soft.h>
```

Bind a function pointer for generic soft constraint feature (PF version)

This function allows one to easily bind a function pointer and corresponding data structure to the soft constraint part *vrna_sc_t* of the *vrna_fold_compound_t*. The function for evaluating the generic soft constraint feature has to return a pseudo free energy \hat{E} as Boltzmann factor, i.e. $\exp(-\hat{E}/kT)$. The required unit for E is *cal/mol*.

See also

[vrna_sc_add_bt\(\)](#), [vrna_sc_add_f\(\)](#), [vrna_sc_add_data\(\)](#)

Parameters

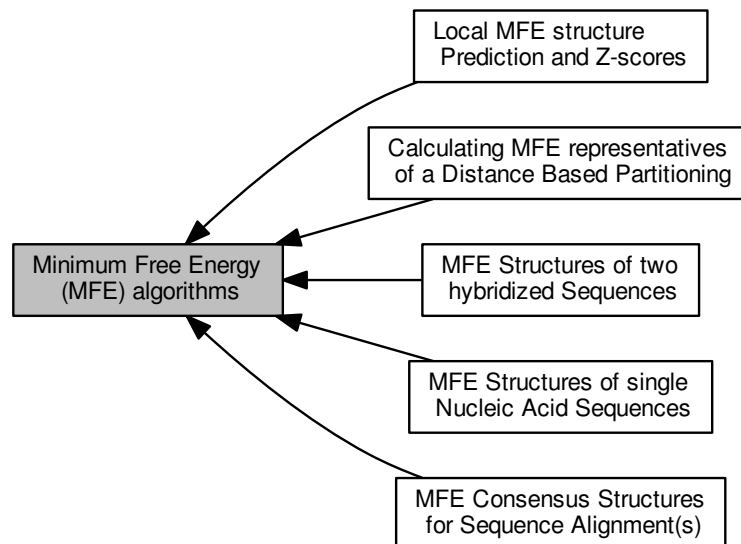
<i>vc</i>	The fold compound the generic soft constraint function should be bound to
<i>exp_f</i>	A pointer to the function that evaluates the generic soft constraint feature

SWIG Wrapper Notes This function is attached as method **sc_add_exp_f()** to objects of type *fold_compound*

15.12 Minimum Free Energy (MFE) algorithms

Compute Minimum Free energy (MFE) and backtrace corresponding secondary structures from RNA sequence data.

Collaboration diagram for Minimum Free Energy (MFE) algorithms:



Modules

- [MFE Consensus Structures for Sequence Alignment\(s\)](#)
- [Calculating MFE representatives of a Distance Based Partitioning](#)

Compute the minimum free energy (MFE) and secondary structures for a partitioning of the secondary structure space according to the base pair distance to two fixed reference structures basepair distance to two fixed reference structures.

- [MFE Structures of single Nucleic Acid Sequences](#)

This module contains all functions and variables related to the calculation of global minimum free energy structures for single sequences.

- [MFE Structures of two hybridized Sequences](#)

*MFE version of cofolding routines This file includes (almost) all function declarations within the **RNALib** that are related to MFE Cofolding... This also includes the Zuker suboptimals calculations, since they are implemented using the cofold routines.*

- [Local MFE structure Prediction and Z-scores](#)

Files

- file [fold.h](#)

MFE calculations for single RNA sequences.

Functions

- float [vrna_mfe](#) ([vrna_fold_compound_t](#) *vc, char *structure)

Compute minimum free energy and an appropriate secondary structure of an RNA sequence, or RNA sequence alignment.

15.12.1 Detailed Description

Compute Minimum Free energy (MFE) and backtrace corresponding secondary structures from RNA sequence data.

The library provides a fast dynamic programming minimum free energy folding algorithm as described in [24]. All relevant parts that directly implement the "Zuker & Stiegler" algorithm for single sequences are described in this section.

Folding of circular RNA sequences is handled as a post-processing step of the forward recursions. See [9] for further details.

Nevertheless, the RNAlib also provides interfaces for the prediction of consensus MFE structures of sequence alignments, MFE structure for two hybridized sequences, local optimal structures and many more. For those more specialized variants of MFE folding routines, please consult the appropriate subsections (Modules) as listed above.

15.12.2 Function Documentation

15.12.2.1 float [vrna_mfe](#) ([vrna_fold_compound_t](#) *vc, char * *structure*)

```
#include <ViennaRNA/mfe.h>
```

Compute minimum free energy and an appropriate secondary structure of an RNA sequence, or RNA sequence alignment.

Depending on the type of the provided [vrna_fold_compound_t](#), this function predicts the MFE for a single sequence, or a corresponding averaged MFE for a sequence alignment. If backtracking is activated, it also constructs the corresponding secondary structure, or consensus structure. Therefore, the second parameter, *structure*, has to point to an allocated block of memory with a size of at least `strlen(sequence) + 1` to store the backtracked MFE structure. (For consensus structures, this is the length of the alignment + 1. If `NULL` is passed, no backtracking will be performed.

Note

This function is polymorphic. It accepts [vrna_fold_compound_t](#) of type [VRNA_FC_TYPE_SINGLE](#), and [VRNA_FC_TYPE_COMPARATIVE](#).

See also

[vrna_fold_compound_t](#), [vrna_fold_compound\(\)](#), [vrna_fold\(\)](#), [vrna_circfold\(\)](#), [vrna_fold_compound_comparative\(\)](#), [vrna_alifold\(\)](#), [vrna_circalifold\(\)](#)

Parameters

<i>vc</i>	fold compound
<i>structure</i>	A pointer to the character array where the secondary structure in dot-bracket notation will be written to (Maybe <code>NULL</code>)

Returns

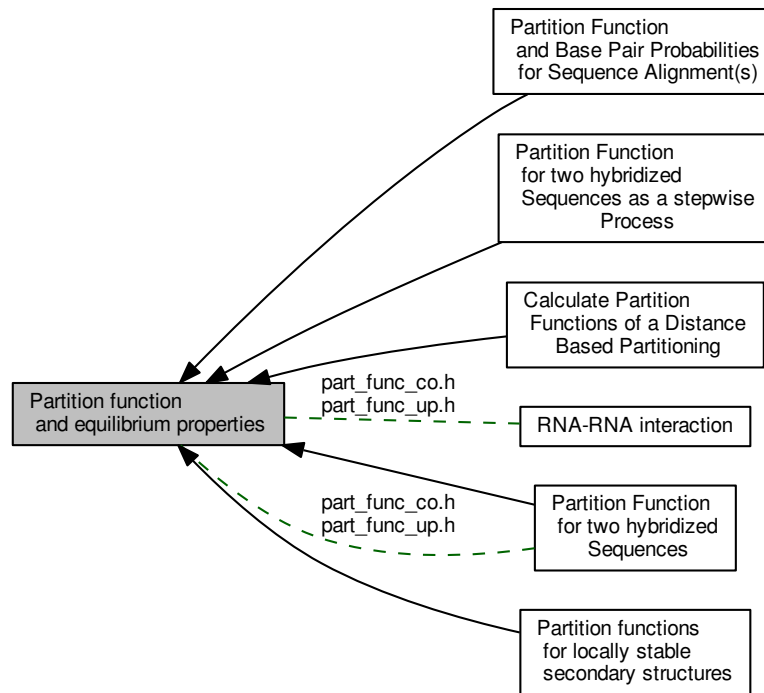
the minimum free energy (MFE) in kcal/mol

SWIG Wrapper Notes This function is attached as method **mfe()** to objects of type *fold_compound*

15.13 Partition function and equilibrium properties

Compute the partition function and various equilibrium properties derived from it.

Collaboration diagram for Partition function and equilibrium properties:



Modules

- [Partition Function and Base Pair Probabilities for Sequence Alignment\(s\)](#)
- [Calculate Partition Functions of a Distance Based Partitioning](#)
Compute the partition function and stochastically sample secondary structures for a partitioning of the secondary structure space according to the base pair distance to two fixed reference structures.
- [Partition Function for two hybridized Sequences](#)
Partition Function Cofolding.
- [Partition Function for two hybridized Sequences as a stepwise Process](#)
RNA-RNA interaction as a stepwise process.
- [Partition functions for locally stable secondary structures](#)

Files

- file [equilibrium_probs.h](#)
Equilibrium Probability implementations.
- file [part_func.h](#)
Partition function implementations.
- file [part_func_co.h](#)
Partition function for two RNA sequences.
- file [part_func_up.h](#)
Implementations for accessibility and RNA-RNA interaction as a stepwise process.

Functions

- double `vrna_mean_bp_distance_pr` (int length, FLT_OR_DBL *pr)
Get the mean base pair distance in the thermodynamic ensemble from a probability matrix.
- double `vrna_mean_bp_distance` (vrna_fold_compound_t *vc)
Get the mean base pair distance in the thermodynamic ensemble.
- vrna_plist_t * `vrna_stack_prob` (vrna_fold_compound_t *vc, double cutoff)
Compute stacking probabilities.
- float `vrna_pf` (vrna_fold_compound_t *vc, char *structure)
Compute the partition function Q for a given RNA sequence, or sequence alignment.
- float `vrna_pf_fold` (const char *sequence, char *structure, vrna_plist_t **pl)
Compute Partition function Q (and base pair probabilities) for an RNA sequence using a comparative method.
- float `vrna_pf_circfold` (const char *sequence, char *structure, vrna_plist_t **pl)
Compute Partition function Q (and base pair probabilities) for a circular RNA sequences using a comparative method.
- float `pf_fold_par` (const char *sequence, char *structure, vrna_exp_param_t *parameters, int calculate_bp↔, int is_constrained, int is_circular)
Compute the partition function Q for a given RNA sequence.
- float `pf_fold` (const char *sequence, char *structure)
Compute the partition function Q of an RNA sequence.
- float `pf_circ_fold` (const char *sequence, char *structure)
Compute the partition function of a circular RNA sequence.
- void `free_pf_arrays` (void)
Free arrays for the partition function recursions.
- void `update_pf_params` (int length)
Recalculate energy parameters.
- void `update_pf_params_par` (int length, vrna_exp_param_t *parameters)
Recalculate energy parameters.
- FLT_OR_DBL * `export_bppm` (void)
*Get a pointer to the base pair probability array
Accessing the base pair probabilities for a pair (i,j) is achieved by.*
- int `get_pf_arrays` (short **S_p, short **S1_p, char **ptype_p, FLT_OR_DBL **qb_p, FLT_OR_DBL **qm↔_p, FLT_OR_DBL **q1k_p, FLT_OR_DBL **qln_p)
Get the pointers to (almost) all relevant computation arrays used in partition function computation.
- double `mean_bp_distance` (int length)
Get the mean base pair distance of the last partition function computation.
- double `mean_bp_distance_pr` (int length, FLT_OR_DBL *pr)
Get the mean base pair distance in the thermodynamic ensemble.
- vrna_plist_t * `vrna_plist_from_probs` (vrna_fold_compound_t *vc, double cut_off)
Create a vrna_plist_t from base pair probability matrix.
- void `assign_plist_from_pr` (vrna_plist_t **pl, FLT_OR_DBL *probs, int length, double cutoff)
Create a vrna_plist_t from a probability matrix.

15.13.1 Detailed Description

Compute the partition function and various equilibrium properties derived from it.

Instead of the minimum free energy structure the partition function of all possible structures and from that the pairing probability for every possible pair can be calculated, using a dynamic programming algorithm as described in [15].

15.13.2 Function Documentation

15.13.2.1 `double vrna_mean_bp_distance_pr (int length, FLT_OR_DBL * pr)`

```
#include <ViennaRNA/equilibrium_probs.h>
```

Get the mean base pair distance in the thermodynamic ensemble from a probability matrix.

$$\langle d \rangle = \sum_{a,b} p_a p_b d(S_a, S_b)$$

this can be computed from the pair probs p_{ij} as

$$\langle d \rangle = \sum_{ij} p_{ij} (1 - p_{ij})$$

Parameters

<i>length</i>	The length of the sequence
<i>pr</i>	The matrix containing the base pair probabilities

Returns

The mean pair distance of the structure ensemble

15.13.2.2 `double vrna_mean_bp_distance (vrna_fold_compound_t * vc)`

```
#include <ViennaRNA/equilibrium_probs.h>
```

Get the mean base pair distance in the thermodynamic ensemble.

$$\langle d \rangle = \sum_{a,b} p_a p_b d(S_a, S_b)$$

this can be computed from the pair probs p_{ij} as

$$\langle d \rangle = \sum_{ij} p_{ij} (1 - p_{ij})$$

Parameters

<i>vc</i>	The fold compound data structure
-----------	----------------------------------

Returns

The mean pair distance of the structure ensemble

SWIG Wrapper Notes This function is attached as method `mean_bp_distance()` to objects of type `fold_compound`

15.13.2.3 `vrna_plist_t* vrna_stack_prob (vrna_fold_compound_t * vc, double cutoff)`

```
#include <ViennaRNA/equilibrium_probs.h>
```

Compute stacking probabilities.

For each possible base pair (i, j) , compute the probability of a stack $(i, j), (i + 1, j - 1)$.

Parameters

<i>vc</i>	The fold compound data structure with precomputed base pair probabilities
<i>cutoff</i>	A cutoff value that limits the output to stacks with $p > \text{cutoff}$.

Returns

A list of stacks with enclosing base pair (i, j) and probability p

15.13.2.4 `float vrna_pf (vrna_fold_compound_t * vc, char * structure)`

```
#include <ViennaRNA/part_func.h>
```

Compute the partition function Q for a given RNA sequence, or sequence alignment.

If *structure* is not a NULL pointer on input, it contains on return a string consisting of the letters ". , | { } ()" denoting bases that are essentially unpaired, weakly paired, strongly paired without preference, weakly upstream (downstream) paired, or strongly up- (down-)stream paired bases, respectively. If the parameter `calculate_bppm` is set to 0 base pairing probabilities will not be computed (saving CPU time), otherwise after calculations took place *pr* will contain the probability that bases i and j pair.

Note

This function is polymorphic. It accepts `vrna_fold_compound_t` of type `VRNA_FC_TYPE_SINGLE`, and `VRNA_FC_TYPE_COMPARATIVE`.

See also

`vrna_fold_compound_t`, `vrna_fold_compound()`, `vrna_pf_fold()`, `vrna_pf_circfold()`, `vrna_fold_compound_comparative()`, `vrna_pf_alifold()`, `vrna_pf_circalifold()`, `vrna_db_from_probs()`, `vrna_exp_params()`, `vrna_aln_pinfo()`

Parameters

<i>in, out</i>	<i>vc</i>	The fold compound data structure
<i>in, out</i>	<i>structure</i>	A pointer to the character array where position-wise pairing propensity will be stored. (Maybe NULL)

Returns

The Gibbs free energy of the ensemble ($G = -RT \cdot \log(Q)$) in kcal/mol

SWIG Wrapper Notes This function is attached as method **pf()** to objects of type *fold_compound*

15.13.2.5 `float vrna_pf_fold (const char * sequence, char * structure, vrna_plist_t ** pl)`

```
#include <ViennaRNA/part_func.h>
```

Compute Partition function Q (and base pair probabilities) for an RNA sequence using a comparative method.

This simplified interface to [vrna_pf\(\)](#) computes the partition function and, if required, base pair probabilities for an RNA sequence using default options. Memory required for dynamic programming (DP) matrices will be allocated and free'd on-the-fly. Hence, after return of this function, the recursively filled matrices are not available any more for any post-processing.

Note

In case you want to use the filled DP matrices for any subsequent post-processing step, or you require other conditions than specified by the default model details, use [vrna_pf\(\)](#), and the data structure [vrna_fold_compound_t](#) instead.

See also

[vrna_pf_circfold\(\)](#), [vrna_pf\(\)](#), [vrna_fold_compound\(\)](#), [vrna_fold_compound_t](#)

Parameters

<i>sequence</i>	RNA sequence
<i>structure</i>	A pointer to the character array where position-wise pairing propensity will be stored. (Maybe NULL)
<i>pl</i>	A pointer to a list of vrna_plist_t to store pairing probabilities (Maybe NULL)

Returns

The Gibbs free energy of the ensemble ($G = -RT \cdot \log(Q)$) in kcal/mol

15.13.2.6 float vrna_pf_circfold (const char * *sequence*, char * *structure*, [vrna_plist_t](#) ** *pl*)

```
#include <ViennaRNA/part_func.h>
```

Compute Partition function Q (and base pair probabilities) for a circular RNA sequences using a comparative method.

This simplified interface to [vrna_pf\(\)](#) computes the partition function and, if required, base pair probabilities for a circular RNA sequence using default options. Memory required for dynamic programming (DP) matrices will be allocated and free'd on-the-fly. Hence, after return of this function, the recursively filled matrices are not available any more for any post-processing.

Note

In case you want to use the filled DP matrices for any subsequent post-processing step, or you require other conditions than specified by the default model details, use [vrna_pf\(\)](#), and the data structure [vrna_fold_compound_t](#) instead.

Folding of circular RNA sequences is handled as a post-processing step of the forward recursions. See [9] for further details.

See also

[vrna_pf_fold\(\)](#), [vrna_pf\(\)](#), [vrna_fold_compound\(\)](#), [vrna_fold_compound_t](#)

Parameters

<i>sequence</i>	A circular RNA sequence
<i>structure</i>	A pointer to the character array where position-wise pairing propensity will be stored. (Maybe NULL)
<i>pl</i>	A pointer to a list of vrna_plist_t to store pairing probabilities (Maybe NULL)

Returns

The Gibbs free energy of the ensemble ($G = -RT \cdot \log(Q)$) in kcal/mol

15.13.2.7 float pf_fold_par (const char * *sequence*, char * *structure*, [vrna_exp_param_t](#) * *parameters*, int *calculate_bppm*, int *is_constrained*, int *is_circular*)

```
#include <ViennaRNA/part\_func.h>
```

Compute the partition function Q for a given RNA sequence.

If *structure* is not a NULL pointer on input, it contains on return a string consisting of the letters ". , | { } () " denoting bases that are essentially unpaired, weakly paired, strongly paired without preference, weakly upstream (downstream) paired, or strongly up- (down-)stream paired bases, respectively. If [fold_constrained](#) is not 0, the *structure* string is interpreted on input as a list of constraints for the folding. The character "x" marks bases that must be unpaired, matching brackets " () " denote base pairs, all other characters are ignored. Any pairs conflicting with the constraint will be forbidden. This is usually sufficient to ensure the constraints are honored. If the parameter *calculate_bppm* is set to 0 base pairing probabilities will not be computed (saving CPU time), otherwise after calculations took place [pr](#) will contain the probability that bases i and j pair.

Deprecated Use [vrna_pf\(\)](#) instead

Note

The global array [pr](#) is deprecated and the user who wants the calculated base pair probabilities for further computations is advised to use the function [export_bppm\(\)](#)

Postcondition

After successful run the hidden folding matrices are filled with the appropriate Boltzmann factors. Depending on whether the global variable [do_backtrack](#) was set the base pair probabilities are already computed and may be accessed for further usage via the [export_bppm\(\)](#) function. A call of [free_pf_arrays\(\)](#) will free all memory allocated by this function. Successive calls will first free previously allocated memory before starting the computation.

See also

[vrna_pf\(\)](#), [bppm_to_structure\(\)](#), [export_bppm\(\)](#), [vrna_exp_params\(\)](#), [free_pf_arrays\(\)](#)

Parameters

in	<i>sequence</i>	The RNA sequence input
in, out	<i>structure</i>	A pointer to a char array where a base pair probability information can be stored in a pseudo-dot-bracket notation (may be NULL, too)
in	<i>parameters</i>	Data structure containing the precalculated Boltzmann factors
in	<i>calculate_bppm</i>	Switch to Base pair probability calculations on/off (0==off)
in	<i>is_constrained</i>	Switch to indicate that a structure constraint is passed via the structure argument (0==off)

Returns

The Gibbs free energy of the ensemble ($G = -RT \cdot \log(Q)$) in kcal/mol

15.13.2.8 float pf_fold (const char * *sequence*, char * *structure*)

```
#include <ViennaRNA/part_func.h>
```

Compute the partition function Q of an RNA sequence.

If *structure* is not a NULL pointer on input, it contains on return a string consisting of the letters ". , | { } () " denoting bases that are essentially unpaired, weakly paired, strongly paired without preference, weakly upstream (downstream) paired, or strongly up- (down-)stream paired bases, respectively. If [fold_constrained](#) is not 0, the *structure* string is interpreted on input as a list of constraints for the folding. The character "x" marks bases that must be unpaired, matching brackets " () " denote base pairs, all other characters are ignored. Any pairs conflicting with the constraint will be forbidden. This is usually sufficient to ensure the constraints are honored. If [do_backtrack](#) has been set to 0 base pairing probabilities will not be computed (saving CPU time), otherwise [pr](#) will contain the probability that bases i and j pair.

Note

The global array [pr](#) is deprecated and the user who wants the calculated base pair probabilities for further computations is advised to use the function [export_bppm\(\)](#).

OpenMP: This function is not entirely threadsafe. While the recursions are working on their own copies of data the model details for the recursions are determined from the global settings just before entering the recursions. Consider using [pf_fold_par\(\)](#) for a really threadsafe implementation.

Precondition

This function takes its model details from the global variables provided in *RNAlib*

Postcondition

After successful run the hidden folding matrices are filled with the appropriate Boltzmann factors. Depending on whether the global variable [do_backtrack](#) was set the base pair probabilities are already computed and may be accessed for further usage via the [export_bppm\(\)](#) function. A call of [free_pf_arrays\(\)](#) will free all memory allocated by this function. Successive calls will first free previously allocated memory before starting the computation.

See also

[pf_fold_par\(\)](#), [pf_circ_fold\(\)](#), [bppm_to_structure\(\)](#), [export_bppm\(\)](#)

Parameters

<i>sequence</i>	The RNA sequence input
<i>structure</i>	A pointer to a char array where a base pair probability information can be stored in a pseudo-dot-bracket notation (may be NULL, too)

Returns

The Gibbs free energy of the ensemble ($G = -RT \cdot \log(Q)$) in kcal/mol

15.13.2.9 float pf_circ_fold (const char * *sequence*, char * *structure*)

```
#include <ViennaRNA/part_func.h>
```

Compute the partition function of a circular RNA sequence.

Note

The global array `pr` is deprecated and the user who wants the calculated base pair probabilities for further computations is advised to use the function `export_bppm()`.

OpenMP: This function is not entirely threadsafe. While the recursions are working on their own copies of data the model details for the recursions are determined from the global settings just before entering the recursions. Consider using `pf_fold_par()` for a really threadsafe implementation.

Precondition

This function takes its model details from the global variables provided in *RNAlib*

Postcondition

After successful run the hidden folding matrices are filled with the appropriate Boltzmann factors. Depending on whether the global variable `do_backtrack` was set the base pair probabilities are already computed and may be accessed for further usage via the `export_bppm()` function. A call of `free_pf_arrays()` will free all memory allocated by this function. Successive calls will first free previously allocated memory before starting the computation.

See also

`vrna_pf()`

Deprecated Use `vrna_pf()` instead!

Parameters

<code>in</code>	<code>sequence</code>	The RNA sequence input
<code>in, out</code>	<code>structure</code>	A pointer to a char array where a base pair probability information can be stored in a pseudo-dot-bracket notation (may be NULL, too)

Returns

The Gibbs free energy of the ensemble ($G = -RT \cdot \log(Q)$) in kcal/mol

15.13.2.10 void free_pf_arrays (void)

```
#include <ViennaRNA/part_func.h>
```

Free arrays for the partition function recursions.

Call this function if you want to free all allocated memory associated with the partition function forward recursion.

Note

Successive calls of `pf_fold()`, `pf_circ_fold()` already check if they should free any memory from a previous run.

OpenMP notice:

This function should be called before leaving a thread in order to avoid leaking memory

Deprecated See `vrna_fold_compound_t` and its related functions for how to free memory occupied by the dynamic programming matrices

Postcondition

All memory allocated by `pf_fold_par()`, `pf_fold()` or `pf_circ_fold()` will be free'd

See also

`pf_fold_par()`, `pf_fold()`, `pf_circ_fold()`

15.13.2.11 void update_pf_params (int *length*)

```
#include <ViennaRNA/part_func.h>
```

Recalculate energy parameters.

Call this function to recalculate the pair matrix and energy parameters after a change in folding parameters like [temperature](#)

Deprecated Use `vrna_exp_params_subst()` instead

15.13.2.12 void update_pf_params_par (int *length*, `vrna_exp_param_t` * *parameters*)

```
#include <ViennaRNA/part_func.h>
```

Recalculate energy parameters.

Deprecated Use `vrna_exp_params_subst()` instead

15.13.2.13 FLT_OR_DBL* export_bppm (void)

```
#include <ViennaRNA/part_func.h>
```

Get a pointer to the base pair probability array

Accessing the base pair probabilities for a pair (i,j) is achieved by.

```
00001 FLT_OR_DBL *pr = export_bppm();
00002 pr_ij          = pr[iindx[i]-j];
```

Precondition

Call [pf_fold_par\(\)](#), [pf_fold\(\)](#) or [pf_circ_fold\(\)](#) first to fill the base pair probability array

See also

[pf_fold\(\)](#), [pf_circ_fold\(\)](#), [vrna_idx_row_wise\(\)](#)

Returns

A pointer to the base pair probability array

15.13.2.14 int get_pf_arrays (short ** S_p, short ** S1_p, char ** ptype_p, FLT_OR_DBL ** qb_p, FLT_OR_DBL ** qm_p, FLT_OR_DBL ** q1k_p, FLT_OR_DBL ** qln_p)

```
#include <ViennaRNA/part_func.h>
```

Get the pointers to (almost) all relevant computation arrays used in partition function computation.

Precondition

In order to assign meaningful pointers, you have to call [pf_fold_par\(\)](#) or [pf_fold\(\)](#) first!

See also

[pf_fold_par\(\)](#), [pf_fold\(\)](#), [pf_circ_fold\(\)](#)

Parameters

out	<i>S_p</i>	A pointer to the 'S' array (integer representation of nucleotides)
out	<i>S1_p</i>	A pointer to the 'S1' array (2nd integer representation of nucleotides)
out	<i>ptype</i> _{← _p}	A pointer to the pair type matrix
out	<i>qb_p</i>	A pointer to the Q ^B matrix
out	<i>qm_p</i>	A pointer to the Q ^M matrix
out	<i>q1k_p</i>	A pointer to the 5' slice of the Q matrix ($q1k(k) = Q(1, k)$)
out	<i>qln_p</i>	A pointer to the 3' slice of the Q matrix ($qln(l) = Q(l, n)$)

Returns

Non Zero if everything went fine, 0 otherwise

15.13.2.15 `double mean_bp_distance (int length)`

```
#include <ViennaRNA/part_func.h>
```

Get the mean base pair distance of the last partition function computation.

Deprecated Use `vrna_mean_bp_distance()` or `vrna_mean_bp_distance_pr()` instead!

See also

`vrna_mean_bp_distance()`, `vrna_mean_bp_distance_pr()`

Parameters

<i>length</i>	
---------------	--

Returns

mean base pair distance in thermodynamic ensemble

15.13.2.16 `double mean_bp_distance_pr (int length, FLT_OR_DBL * pr)`

```
#include <ViennaRNA/part_func.h>
```

Get the mean base pair distance in the thermodynamic ensemble.

This is a threadsafe implementation of `mean_bp_dist()` !

$$\langle d \rangle = \sum_{a,b} p_a p_b d(S_a, S_b)$$

this can be computed from the pair probs p_{ij} as

$$\langle d \rangle = \sum_{ij} p_{ij} (1 - p_{ij})$$

Deprecated Use `vrna_mean_bp_distance()` or `vrna_mean_bp_distance_pr()` instead!

Parameters

<i>length</i>	The length of the sequence
<i>pr</i>	The matrix containing the base pair probabilities

Returns

The mean pair distance of the structure ensemble

15.13.2.17 `vrna_plist_t* vrna_plist_from_probs (vrna_fold_compound_t * vc, double cut_off)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a `vrna_plist_t` from base pair probability matrix.

The probability matrix provided via the `vrna_fold_compound_t` is parsed and all pair probabilities above the given threshold are used to create an entry in the plist

The end of the plist is marked by sequence positions *i* as well as *j* equal to 0. This condition should be used to stop looping over its entries

Parameters

in	<i>vc</i>	The fold compound
in	<i>cut_off</i>	The cutoff value

Returns

A pointer to the plist that is to be created

15.13.2.18 `void assign_plist_from_pr (vrna_plist_t ** pl, FLT_OR_DBL * probs, int length, double cutoff)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a `vrna_plist_t` from a probability matrix.

The probability matrix given is parsed and all pair probabilities above the given threshold are used to create an entry in the plist

The end of the plist is marked by sequence positions *i* as well as *j* equal to 0. This condition should be used to stop looping over its entries

Note

This function is threadsafe

Deprecated Use `vrna_plist_from_probs()` instead!

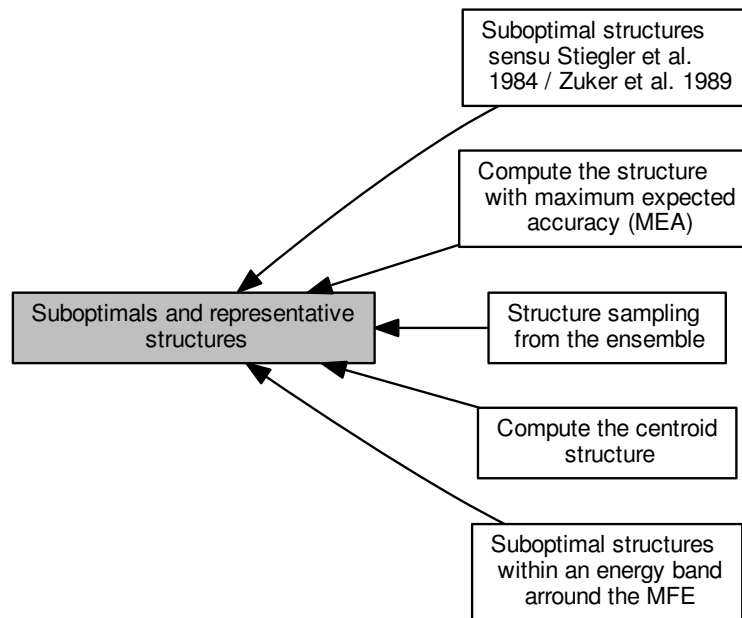
Parameters

out	<i>pl</i>	A pointer to the <code>vrna_plist_t</code> that is to be created
in	<i>probs</i>	The probability matrix used for creating the plist
in	<i>length</i>	The length of the RNA sequence
in	<i>cutoff</i>	The cutoff value

15.14 Suboptimals and representative structures

Sample and enumerate suboptimal secondary structures from RNA sequence data.

Collaboration diagram for Suboptimals and representative structures:



Modules

- [Suboptimal structures sensu Stiegler et al. 1984 / Zuker et al. 1989](#)
- [Suboptimal structures within an energy band around the MFE](#)
- [Structure sampling from the ensemble](#)
- [Compute the structure with maximum expected accuracy \(MEA\)](#)
- [Compute the centroid structure](#)

Files

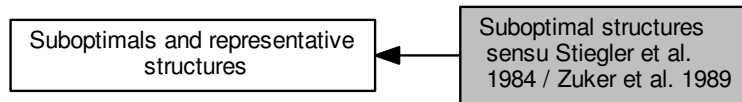
- file [boltzmann_sampling.h](#)
Boltzmann Sampling of secondary structures from the ensemble.
- file [centroid.h](#)
Centroid structure computation.
- file [MEA.h](#)
Computes a MEA (maximum expected accuracy) structure.
- file [mm.h](#)
Several Maximum Matching implementations.
- file [subopt.h](#)
RNAsubopt and density of states declarations.

15.14.1 Detailed Description

Sample and enumerate suboptimal secondary structures from RNA sequence data.

15.15 Suboptimal structures sensu Stiegler et al. 1984 / Zuker et al. 1989

Collaboration diagram for Suboptimal structures sensu Stiegler et al. 1984 / Zuker et al. 1989:



Functions

- `vrna_subopt_solution_t * vrna_subopt_zuker (vrna_fold_compound_t *vc)`
Compute Zuker type suboptimal structures.
- `SOLUTION * zukersubopt (const char *string)`
Compute Zuker type suboptimal structures.
- `SOLUTION * zukersubopt_par (const char *string, vrna_param_t *parameters)`
Compute Zuker type suboptimal structures.

15.15.1 Detailed Description

15.15.2 Function Documentation

15.15.2.1 `vrna_subopt_solution_t * vrna_subopt_zuker (vrna_fold_compound_t * vc)`

```
#include <ViennaRNA/subopt.h>
```

Compute Zuker type suboptimal structures.

Compute Suboptimal structures according to M. Zuker [23] , i.e. for every possible base pair the minimum energy structure containing the resp. base pair. Returns a list of these structures and their energies.

Note

This function internally uses the cofold implementation to compute the suboptimal structures. For that purpose, the function doubles the sequence and enlarges the DP matrices, which in fact will grow by a factor of 4 during the computation! At the end of the structure prediction, everything will be re-set to its original requirements, i.e. normal sequence, normal (empty) DP matrices.

Bug Due to resizing, any pre-existing constraints will be lost!

See also

[vrna_subopt\(\)](#), [zukersubopt\(\)](#), [zukersubopt_par\(\)](#)

Parameters

<code>vc</code>	fold compound
-----------------	---------------

Returns

List of zucker suboptimal structures

SWIG Wrapper Notes This function is attached as method **subopt_zucker()** to objects of type *fold_compound*

15.15.2.2 SOLUTION* zuckersubopt (const char * *string*)

```
#include <ViennaRNA/subopt.h>
```

Compute Zuker type suboptimal structures.

Compute Suboptimal structures according to M. Zuker, i.e. for every possible base pair the minimum energy structure containing the resp. base pair. Returns a list of these structures and their energies.

Deprecated use `vrna_zuckersubopt()` instead

Parameters

<i>string</i>	RNA sequence
---------------	--------------

Returns

List of zucker suboptimal structures

15.15.2.3 SOLUTION* zuckersubopt_par (const char * *string*, vrna_param_t * *parameters*)

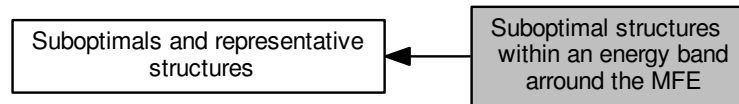
```
#include <ViennaRNA/subopt.h>
```

Compute Zuker type suboptimal structures.

Deprecated use `vrna_zuckersubopt()` instead

15.16 Suboptimal structures within an energy band around the MFE

Collaboration diagram for Suboptimal structures within an energy band around the MFE:



Typedefs

- typedef void([vrna_subopt_callback](#)) (const char *structure, float energy, void *data)
Callback for [vrna_subopt_cb\(\)](#)

Functions

- [vrna_subopt_solution_t](#) * [vrna_subopt](#) ([vrna_fold_compound_t](#) *vc, int delta, int sorted, FILE *fp)
Returns list of subopt structures or writes to fp.
- void [vrna_subopt_cb](#) ([vrna_fold_compound_t](#) *vc, int delta, [vrna_subopt_callback](#) *cb, void *data)
Generate suboptimal structures within an energy band around the MFE.
- [SOLUTION](#) * [subopt](#) (char *seq, char *structure, int delta, FILE *fp)
Returns list of subopt structures or writes to fp.
- [SOLUTION](#) * [subopt_par](#) (char *seq, char *structure, [vrna_param_t](#) *parameters, int delta, int is_↔constrained, int is_circular, FILE *fp)
Returns list of subopt structures or writes to fp.
- [SOLUTION](#) * [subopt_circ](#) (char *seq, char *sequence, int delta, FILE *fp)
Returns list of circular subopt structures or writes to fp.

Variables

- double [print_energy](#)
printing threshold for use with logML
- int [subopt_sorted](#)
Sort output by energy.

15.16.1 Detailed Description

15.16.2 Function Documentation

15.16.2.1 `vrna_subopt_solution_t * vrna_subopt (vrna_fold_compound_t * vc, int delta, int sorted, FILE * fp)`

```
#include <ViennaRNA/subopt.h>
```

Returns list of subopt structures or writes to fp.

This function produces **all** suboptimal secondary structures within 'delta' * 0.01 kcal/mol of the optimum, see [21]. The results are either directly written to a 'fp' (if 'fp' is not NULL), or (fp==NULL) returned in a `vrna_subopt_solution_t *` list terminated by an entry where the 'structure' member is NULL.

Note

This function requires all multibranch loop DP matrices for unique multibranch loop backtracing. Therefore, the supplied `vrna_fold_compound_t` `vc` (argument 1) must be initialized with `vrna_md_t.uniq_ML = 1`, for instance like this:

```
00001 vrna_md_t md;
00002 vrna_md_set_default (&md);
00003 md.uniq_ML = 1;
00004
00005 vrna_fold_compound_t *vc=vrna_fold_compound("GGGGGGAAAAAACCCCCC", &md, VRNA_OPTION_DEFAULT);
```

See also

[vrna_subopt_cb\(\)](#), [vrna_subopt_zuker\(\)](#)

Parameters

<i>vc</i>	
<i>delta</i>	
<i>sorted</i>	Sort results by energy in ascending order
<i>fp</i>	

Returns

SWIG Wrapper Notes This function is attached as method `subopt()` to objects of type `fold_compound`

15.16.2.2 `void vrna_subopt_cb (vrna_fold_compound_t * vc, int delta, vrna_subopt_callback * cb, void * data)`

```
#include <ViennaRNA/subopt.h>
```

Generate suboptimal structures within an energy band around the MFE.

This is the most generic implementation of the suboptimal structure generator according to Wuchty et al. 1999 [21]. Identical to `vrna_subopt()`, it computes all secondary structures within an energy band `delta` around the MFE. However, this function does not print the resulting structures and their corresponding free energies to a file pointer, or returns them as a list. Instead, it calls a user-provided callback function which it passes the structure in dot-bracket format, the corresponding free energy in kcal/mol, and a user-provided data structure each time a structure was backtracked successfully. This function indicates the final output, i.e. the end of the backtracking procedure by passing NULL instead of an actual dot-bracket string to the callback.

Note

This function requires all multibranch loop DP matrices for unique multibranch loop backtracing. Therefore, the supplied `vrna_fold_compound_t` `vc` (argument 1) must be initialized with `vrna_md_t.uniq_ML = 1`, for instance like this:

```
00001 vrna_md_t md;
00002 vrna_md_set_default(&md);
00003 md.uniq_ML = 1;
00004
00005 vrna_fold_compound_t *vc=vrna_fold_compound("GGGGGGAAAAAACCCCC", &md, VRNA_OPTION_DEFAULT);
```

See also

[vrna_subopt_callback](#), [vrna_subopt\(\)](#), [vrna_subopt_zuker\(\)](#)

Parameters

<i>vc</i>	fold compound with the sequence data
<i>delta</i>	Energy band around the MFE in 10cal/mol, i.e. deka-calories
<i>cb</i>	Pointer to a callback function that handles the backtracked structure and its free energy in kcal/mol
<i>data</i>	Pointer to some data structure that is passed along to the callback

SWIG Wrapper Notes This function is attached as method **subopt_cb()** to objects of type *fold_compound*

15.16.2.3 SOLUTION* `subopt (char * seq, char * structure, int delta, FILE * fp)`

```
#include <ViennaRNA/subopt.h>
```

Returns list of subopt structures or writes to fp.

This function produces **all** suboptimal secondary structures within 'delta' * 0.01 kcal/mol of the optimum. The results are either directly written to a 'fp' (if 'fp' is not NULL), or (fp==NULL) returned in a **SOLUTION** * list terminated by an entry where the 'structure' pointer is NULL.

Parameters

<i>seq</i>	
<i>structure</i>	
<i>delta</i>	
<i>fp</i>	

Returns

15.16.2.4 SOLUTION* `subopt_circ (char * seq, char * sequence, int delta, FILE * fp)`

```
#include <ViennaRNA/subopt.h>
```

Returns list of circular subopt structures or writes to fp.

This function is similar to [subopt\(\)](#) but calculates secondary structures assuming the RNA sequence to be circular instead of linear

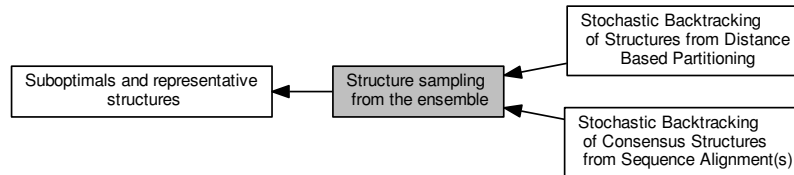
Parameters

<i>seq</i>	
<i>sequence</i>	
<i>delta</i>	
<i>fp</i>	

Returns

15.17 Structure sampling from the ensemble

Collaboration diagram for Structure sampling from the ensemble:



Modules

- [Stochastic Backtracking of Consensus Structures from Sequence Alignment\(s\)](#)
- [Stochastic Backtracking of Structures from Distance Based Partitioning](#)

Contains functions related to stochastic backtracking from a specified distance class.

Functions

- `char * vrna_pbacktrack5 (vrna_fold_compound_t *vc, int length)`
Sample a secondary structure of a subsequence from the Boltzmann ensemble according its probability.
- `char * vrna_pbacktrack (vrna_fold_compound_t *vc)`
Sample a secondary structure (consensus structure) from the Boltzmann ensemble according its probability.
- `char * pbacktrack (char *sequence)`
Sample a secondary structure from the Boltzmann ensemble according its probability.
- `char * pbacktrack_circ (char *sequence)`
Sample a secondary structure of a circular RNA from the Boltzmann ensemble according its probability.

Variables

- `int st_back`
Flag indicating that auxiliary arrays are needed throughout the computations. This is essential for stochastic backtracking.

15.17.1 Detailed Description

15.17.2 Function Documentation

15.17.2.1 `char* vrna_pbacktrack5 (vrna_fold_compound_t * vc, int length)`

```
#include <ViennaRNA/boltzmann_sampling.h>
```

Sample a secondary structure of a subsequence from the Boltzmann ensemble according its probability.

Precondition

The fold compound has to be obtained using the [VRNA_OPTION_HYBRID](#) option in `vrna_fold_compound()` `vrna_pf()` has to be called first to fill the partition function matrices

Parameters

<i>vc</i>	The fold compound data structure
<i>length</i>	The length of the subsequence to consider (starting with 5' end)

Returns

A sampled secondary structure in dot-bracket notation

15.17.2.2 `char* vrna_pbacktrack (vrna_fold_compound_t * vc)`

```
#include <ViennaRNA/boltzmann_sampling.h>
```

Sample a secondary structure (consensus structure) from the Boltzmann ensemble according its probability.

Precondition

The dynamic programming (DP) matrices have to allow for unique multibranch loop decomposition, i.e. the `vrna_md_t.uniq_ML` flag has to be non-zero before calling `vrna_fold_compound()`
`vrna_pf()` has to be called first to fill the partition function matrices

Note

This function is polymorphic. It accepts `vrna_fold_compound_t` of type `VRNA_FC_TYPE_SINGLE`, and `VRNA_FC_TYPE_COMPARATIVE`.
The function will automagically detect cicular RNAs based on the `model_details` in `exp_params` as provided via the `vrna_fold_compound_t`

Parameters

<i>vc</i>	The fold compound data structure
-----------	----------------------------------

Returns

A sampled secondary structure in dot-bracket notation

15.17.2.3 `char* pbacktrack (char * sequence)`

```
#include <ViennaRNA/part_func.h>
```

Sample a secondary structure from the Boltzmann ensemble according its probability.

Precondition

`st_back` has to be set to 1 before calling `pf_fold()` or `pf_fold_par()`
`pf_fold_par()` or `pf_fold()` have to be called first to fill the partition function matrices

Parameters

<i>sequence</i>	The RNA sequence
-----------------	------------------

Returns

A sampled secondary structure in dot-bracket notation

15.17.2.4 `char* pbacktrack_circ (char * sequence)`

```
#include <ViennaRNA/part_func.h>
```

Sample a secondary structure of a circular RNA from the Boltzmann ensemble according its probability.

This function does the same as [pbacktrack\(\)](#) but assumes the RNA molecule to be circular

Precondition

[st_back](#) has to be set to 1 before calling [pf_fold\(\)](#) or [pf_fold_par\(\)](#)
[pf_fold_par\(\)](#) or [pf_circ_fold\(\)](#) have to be called first to fill the partition function matrices

Deprecated Use [vrna_pbacktrack\(\)](#) instead.

Parameters

<i>sequence</i>	The RNA sequence
-----------------	------------------

Returns

A sampled secondary structure in dot-bracket notation

15.17.3 Variable Documentation

15.17.3.1 `int st_back`

```
#include <ViennaRNA/part_func.h>
```

Flag indicating that auxiliary arrays are needed throughout the computations. This is essential for stochastic backtracking.

Set this variable to 1 prior to a call of [pf_fold\(\)](#) to ensure that all matrices needed for stochastic backtracking are filled in the forward recursions

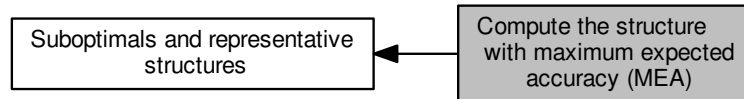
Deprecated set the *uniq_ML* flag in [vrna_md_t](#) before passing it to [vrna_fold_compound\(\)](#).

See also

[pbacktrack\(\)](#), [pbacktrack_circ](#)

15.18 Compute the structure with maximum expected accuracy (MEA)

Collaboration diagram for Compute the structure with maximum expected accuracy (MEA):



Functions

- float [MEA](#) ([plist](#) *p, char *structure, double gamma)
Computes a MEA (maximum expected accuracy) structure.

15.18.1 Detailed Description

15.18.2 Function Documentation

15.18.2.1 float MEA ([plist](#) * p, char * *structure*, double *gamma*)

```
#include <ViennaRNA/MEA.h>
```

Computes a MEA (maximum expected accuracy) structure.

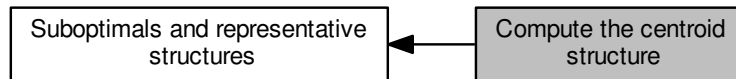
The algorithm maximizes the expected accuracy

$$A(S) = \sum_{(i,j) \in S} 2\gamma p_{ij} + \sum_{i \notin S} p_i^u$$

Higher values of γ result in more base pairs of lower probability and thus higher sensitivity. Low values of γ result in structures containing only highly likely pairs (high specificity). The code of the MEA function also demonstrates the use of sparse dynamic programming scheme to reduce the time and memory complexity of folding.

15.19 Compute the centroid structure

Collaboration diagram for Compute the centroid structure:



Functions

- `char * vrna_centroid (vrna_fold_compound_t *vc, double *dist)`
Get the centroid structure of the ensemble.
- `char * vrna_centroid_from_plist (int length, double *dist, vrna_plist_t *pl)`
Get the centroid structure of the ensemble.
- `char * vrna_centroid_from_probs (int length, double *dist, FLT_OR_DBL *probs)`
Get the centroid structure of the ensemble.

15.19.1 Detailed Description

15.19.2 Function Documentation

15.19.2.1 `char* vrna_centroid (vrna_fold_compound_t * vc, double * dist)`

```
#include <ViennaRNA/centroid.h>
```

Get the centroid structure of the ensemble.

The centroid is the structure with the minimal average distance to all other structures

$$\langle d(S) \rangle = \sum_{(i,j) \in S} (1 - p_{ij}) + \sum_{(i,j) \notin S} p_{ij}$$

Thus, the centroid is simply the structure containing all pairs with $p_{ij} > 0.5$. The distance of the centroid to the ensemble is written to the memory addressed by *dist*.

Parameters

in	<i>vc</i>	The fold compound data structure
out	<i>dist</i>	A pointer to the distance variable where the centroid distance will be written to

Returns

The centroid structure of the ensemble in dot-bracket notation

15.19.2.2 `char* vrna_centroid_from_plist (int length, double * dist, vrna_plist_t * pl)`

```
#include <ViennaRNA/centroid.h>
```

Get the centroid structure of the ensemble.

This function is a threadsafe replacement for `centroid()` with a `vrna_plist_t` input

The centroid is the structure with the minimal average distance to all other structures

$$\langle d(S) \rangle = \sum_{(i,j) \in S} (1 - p_{ij}) + \sum_{(i,j) \notin S} p_{ij}$$

Thus, the centroid is simply the structure containing all pairs with $p_{ij} > 0.5$. The distance of the centroid to the ensemble is written to the memory addressed by *dist*.

Parameters

in	<i>length</i>	The length of the sequence
out	<i>dist</i>	A pointer to the distance variable where the centroid distance will be written to
in	<i>pl</i>	A pair list containing base pair probability information about the ensemble

Returns

The centroid structure of the ensemble in dot-bracket notation

15.19.2.3 `char* vrna_centroid_from_probs (int length, double * dist, FLT_OR_DBL * probs)`

```
#include <ViennaRNA/centroid.h>
```

Get the centroid structure of the ensemble.

This function is a threadsafe replacement for `centroid()` with a probability array input

The centroid is the structure with the minimal average distance to all other structures

$$\langle d(S) \rangle = \sum_{(i,j) \in S} (1 - p_{ij}) + \sum_{(i,j) \notin S} p_{ij}$$

Thus, the centroid is simply the structure containing all pairs with $p_{ij} > 0.5$. The distance of the centroid to the ensemble is written to the memory addressed by *dist*.

Parameters

in	<i>length</i>	The length of the sequence
out	<i>dist</i>	A pointer to the distance variable where the centroid distance will be written to
in	<i>probs</i>	An upper triangular matrix containing base pair probabilities (access via <code>iindx_vrna_idx_row_wise()</code>)

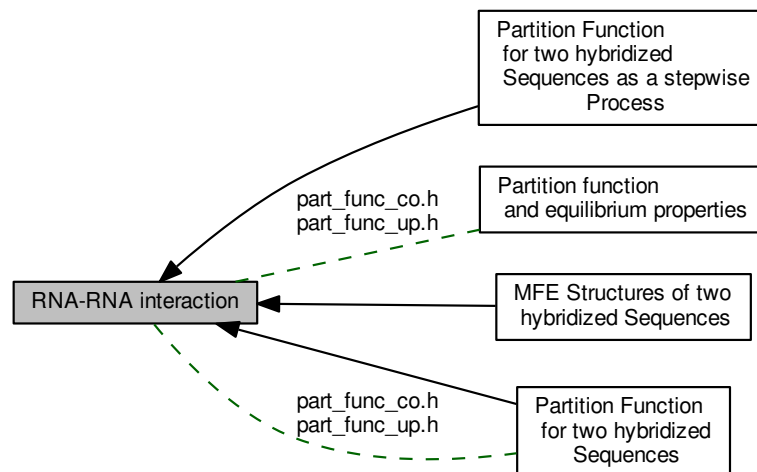
Returns

The centroid structure of the ensemble in dot-bracket notation

15.20 RNA-RNA interaction

Predict structures formed by two molecules upon hybridization.

Collaboration diagram for RNA-RNA interaction:



Modules

- [MFE Structures of two hybridized Sequences](#)

*MFE version of cofolding routines This file includes (almost) all function declarations within the **RNALib** that are related to MFE Cofolding... This also includes the Zuker suboptimals calculations, since they are implemented using the cofold routines.*

- [Partition Function for two hybridized Sequences](#)

Partition Function Cofolding.

- [Partition Function for two hybridized Sequences as a stepwise Process](#)

RNA-RNA interaction as a stepwise process.

Files

- file [cofold.h](#)

MFE implementations for RNA-RNA interaction.

- file [duplex.h](#)

Functions for simple RNA-RNA duplex interactions.

- file [part_func_co.h](#)

Partition function for two RNA sequences.

- file [part_func_up.h](#)

Implementations for accessibility and RNA-RNA interaction as a stepwise process.

15.20.1 Detailed Description

Predict structures formed by two molecules upon hybridization.

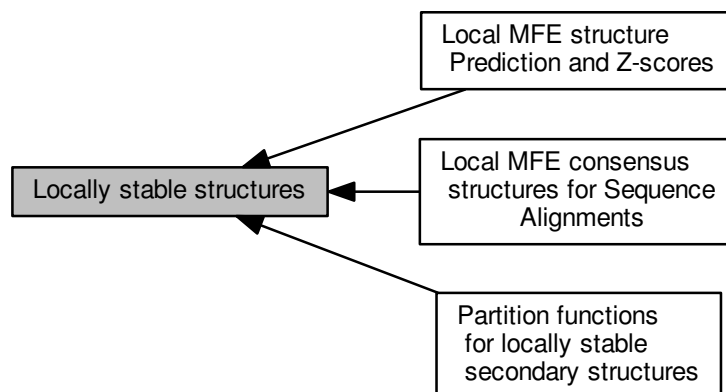
The function of an RNA molecule often depends on its interaction with other RNAs. The following routines therefore allows one to predict structures formed by two RNA molecules upon hybridization.

One approach to co-folding two RNAs consists of concatenating the two sequences and keeping track of the concatenation point in all energy evaluations. Correspondingly, many of the [cofold\(\)](#) and [co_pf_fold\(\)](#) routines below take one sequence string as argument and use the the global variable [cut_point](#) to mark the concatenation point. Note that while the *RNAcofold* program uses the '&' character to mark the chain break in its input, you should not use an '&' when using the library routines (set [cut_point](#) instead).

In a second approach to co-folding two RNAs, cofolding is seen as a stepwise process. In the first step the probability of an unpaired region is calculated and in a second step this probability of an unpaired region is multiplied with the probability of an interaction between the two RNAs. This approach is implemented for the interaction between a long target sequence and a short ligand RNA. Function [pf_unstru\(\)](#) calculates the partition function over all unpaired regions in the input sequence. Function [pf_interact\(\)](#), which calculates the partition function over all possible interactions between two sequences, needs both sequence as separate strings as input.

15.21 Locally stable structures

Collaboration diagram for Locally stable structures:



Modules

- [Local MFE structure Prediction and Z-scores](#)
- [Partition functions for locally stable secondary structures](#)
- [Local MFE consensus structures for Sequence Alignments](#)

Files

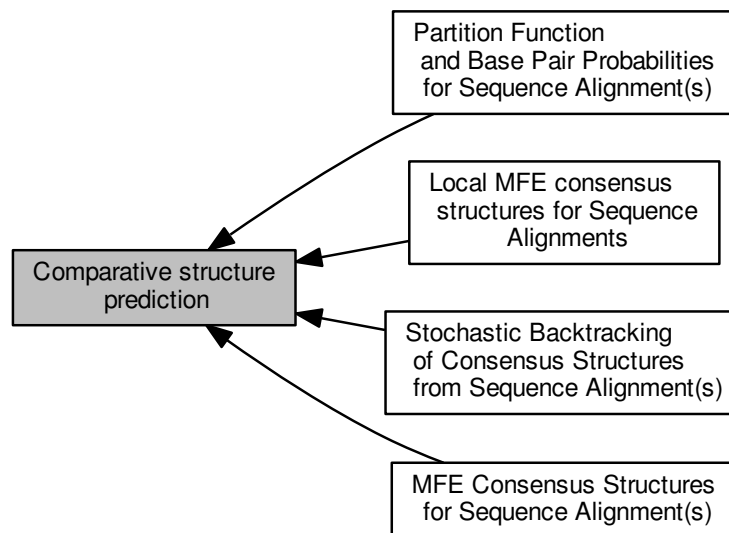
- file [Lfold.h](#)
Functions for locally optimal MFE structure prediction.
- file [LPfold.h](#)
Partition function implementation for the Lfold algorithm.

15.21.1 Detailed Description

15.22 Comparative structure prediction

compute various properties (consensus MFE structures, partition function, Boltzmann distributed stochastic samples, ...) for RNA sequence alignments

Collaboration diagram for Comparative structure prediction:



Modules

- [MFE Consensus Structures for Sequence Alignment\(s\)](#)
- [Partition Function and Base Pair Probabilities for Sequence Alignment\(s\)](#)
- [Stochastic Backtracking of Consensus Structures from Sequence Alignment\(s\)](#)
- [Local MFE consensus structures for Sequence Alignments](#)

Files

- file [alifold.h](#)
Functions for comparative structure prediction using RNA sequence alignments.

Functions

- float [energy_of_alistruct](#) (const char **sequences, const char *structure, int n_seq, float *energy)
Calculate the free energy of a consensus structure given a set of aligned sequences.
- int [get_alipf_arrays](#) (short ***S_p, short ***S5_p, short ***S3_p, unsigned short ***a2s_p, char ***Ss←_p, [FLT_OR_DBL](#) **qb_p, [FLT_OR_DBL](#) **qm_p, [FLT_OR_DBL](#) **q1k_p, [FLT_OR_DBL](#) **qln_p, short **pscore)
Get pointers to (almost) all relevant arrays used in alifold's partition function computation.
- void [update_alifold_params](#) (void)
Update the energy parameters for alifold function.

Variables

- double `cv_fact`
This variable controls the weight of the covariance term in the energy function of alignment folding algorithms.
- double `nc_fact`
This variable controls the magnitude of the penalty for non-compatible sequences in the covariance term of alignment folding algorithms.
- int `vrna_aln_mpi` (const char **alignment)
Get the mean pairwise identity in steps from ?to?(ident)
- int `get_mpi` (char *Aseq[], int n_seq, int length, int *mini)
Get the mean pairwise identity in steps from ?to?(ident)
- void `encode_ali_sequence` (const char *sequence, short *S, short *s5, short *s3, char *ss, unsigned short *as, int circ)
Get arrays with encoded sequence of the alignment.
- void `alloc_sequence_arrays` (const char **sequences, short ***S, short ***S5, short ***S3, unsigned short ***a2s, char ***Ss, int circ)
Allocate memory for sequence array used to deal with aligned sequences.
- void `free_sequence_arrays` (unsigned int n_seq, short ***S, short ***S5, short ***S3, unsigned short ***a2s, char ***Ss)
Free the memory of the sequence arrays used to deal with aligned sequences.
- float ** `get_ribosum` (const char **Aseq, int n_seq, int length)
Retrieve a RiboSum Scoring Matrix for a given Alignment.
- float ** `readribosum` (char *name)
Read a RiboSum or other user-defined Scoring Matrix and Store into global Memory.

15.22.1 Detailed Description

compute various properties (consensus MFE structures, partition function, Boltzmann distributed stochastic samples, ...) for RNA sequence alignments

Consensus structures can be predicted by a modified version of the `fold()` algorithm that takes a set of aligned sequences instead of a single sequence. The energy function consists of the mean energy averaged over the sequences, plus a covariance term that favors pairs with consistent and compensatory mutations and penalizes pairs that cannot be formed by all structures. For details see [7] and [1].

15.22.2 Function Documentation

15.22.2.1 float `energy_of_alistruct` (const char ** *sequences*, const char * *structure*, int *n_seq*, float * *energy*)

```
#include <ViennaRNA/alifold.h>
```

Calculate the free energy of a consensus structure given a set of aligned sequences.

Deprecated Usage of this function is discouraged! Use `vrna_eval_structure()`, and `vrna_eval_covar_structure()` instead!

Parameters

<i>sequences</i>	The NULL terminated array of sequences
<i>structure</i>	The consensus structure
<i>n_seq</i>	The number of sequences in the alignment
<i>energy</i>	A pointer to an array of at least two floats that will hold the free energies (energy[0] will contain the free energy, energy[1] will be filled with the covariance energy term)

Returns

free energy in kcal/mol

15.22.2.2 `int get_alipf_arrays (short *** S_p, short *** S5_p, short *** S3_p, unsigned short *** a2s_p, char *** Ss_p, FLT_OR_DBL ** qb_p, FLT_OR_DBL ** qm_p, FLT_OR_DBL ** q1k_p, FLT_OR_DBL ** qln_p, short ** pscore)`

```
#include <ViennaRNA/alifold.h>
```

Get pointers to (almost) all relevant arrays used in alifold's partition function computation.

Note

To obtain meaningful pointers, call `alipf_fold` first!

See also

`pf_alifold()`, [alipf_circ_fold\(\)](#)

Deprecated It is discouraged to use this function! The new [vrna_fold_compound_t](#) allows direct access to all necessary consensus structure prediction related variables!

See also

[vrna_fold_compound_t](#), [vrna_fold_compound_comparative\(\)](#), [vrna_pf\(\)](#)

Parameters

<i>S_p</i>	A pointer to the 'S' array (integer representation of nucleotides)
<i>S5_p</i>	A pointer to the 'S5' array
<i>S3_p</i>	A pointer to the 'S3' array
<i>a2s↔ _p</i>	A pointer to the pair type matrix
<i>Ss_p</i>	A pointer to the 'Ss' array
<i>qb_p</i>	A pointer to the Q^B matrix
<i>qm_p</i>	A pointer to the Q^M matrix
<i>q1k↔ _p</i>	A pointer to the 5' slice of the Q matrix ($q1k(k) = Q(1, k)$)
<i>qln_p</i>	A pointer to the 3' slice of the Q matrix ($qln(l) = Q(l, n)$)
<i>pscore</i>	A pointer to the start of a pscore list

Returns

Non Zero if everything went fine, 0 otherwise

15.22.2.3 void update_alifold_params (void)

```
#include <ViennaRNA/alifold.h>
```

Update the energy parameters for alifold function.

Call this to recalculate the pair matrix and energy parameters after a change in folding parameters like [temperature](#)

Deprecated Usage of this function is discouraged! The new API uses [vrna_fold_compound_t](#) to lump all folding related necessities together, including the energy parameters. Use [vrna_update_fold_params\(\)](#) to update the energy parameters within a [vrna_fold_compound_t](#).

15.22.2.4 int vrna_aln_mpi (const char ** alignment)

```
#include <ViennaRNA/aln_util.h>
```

Get the mean pairwise identity in steps from ?to?(ident)

Parameters

<i>alignment</i>	Aligned sequences
------------------	-------------------

Returns

The mean pairwise identity

15.22.2.5 int get_mpi (char * Aseq[], int n_seq, int length, int * mini)

```
#include <ViennaRNA/aln_util.h>
```

Get the mean pairwise identity in steps from ?to?(ident)

Deprecated Use [vrna_aln_mpi\(\)](#) as a replacement

Parameters

<i>Aseq</i>	
<i>n_seq</i>	The number of sequences in the alignment
<i>length</i>	The length of the alignment
<i>mini</i>	

Returns

The mean pairwise identity

15.22.2.6 `void encode_aln_sequence (const char * sequence, short * S, short * s5, short * s3, char * ss, unsigned short * as, int circ)`

```
#include <ViennaRNA/aln_util.h>
```

Get arrays with encoded sequence of the alignment.

this function assumes that in *S*, *S5*, *s3*, *ss* and *as* enough space is already allocated (size must be at least sequence length+2)

Parameters

<i>sequence</i>	The gapped sequence from the alignment
<i>S</i>	pointer to an array that holds encoded sequence
<i>s5</i>	pointer to an array that holds the next base 5' of alignment position i
<i>s3</i>	pointer to an array that holds the next base 3' of alignment position i
<i>ss</i>	
<i>as</i>	
<i>circ</i>	assume the molecules to be circular instead of linear (circ=0)

15.22.2.7 `void alloc_sequence_arrays (const char ** sequences, short *** S, short *** S5, short *** S3, unsigned short *** a2s, char *** Ss, int circ)`

```
#include <ViennaRNA/aln_util.h>
```

Allocate memory for sequence array used to deal with aligned sequences.

Note that these arrays will also be initialized according to the sequence alignment given

See also

[free_sequence_arrays\(\)](#)

Parameters

<i>sequences</i>	The aligned sequences
<i>S</i>	A pointer to the array of encoded sequences
<i>S5</i>	A pointer to the array that contains the next 5' nucleotide of a sequence position
<i>S3</i>	A pointer to the array that contains the next 3' nucleotide of a sequence position
<i>a2s</i>	A pointer to the array that contains the alignment to sequence position mapping
<i>Ss</i>	A pointer to the array that contains the ungapped sequence
<i>circ</i>	assume the molecules to be circular instead of linear (circ=0)

15.22.2.8 `void free_sequence_arrays (unsigned int n_seq, short *** S, short *** S5, short *** S3, unsigned short *** a2s, char *** Ss)`

```
#include <ViennaRNA/aln_util.h>
```

Free the memory of the sequence arrays used to deal with aligned sequences.

This function frees the memory previously allocated with [alloc_sequence_arrays\(\)](#)

See also

[alloc_sequence_arrays\(\)](#)

Parameters

<i>n_seq</i>	The number of aligned sequences
<i>S</i>	A pointer to the array of encoded sequences
<i>S5</i>	A pointer to the array that contains the next 5' nucleotide of a sequence position
<i>S3</i>	A pointer to the array that contains the next 3' nucleotide of a sequence position
<i>a2s</i>	A pointer to the array that contains the alignment to sequence position mapping
<i>Ss</i>	A pointer to the array that contains the ungapped sequence

15.22.3 Variable Documentation

15.22.3.1 `double cv_fact`

```
#include <ViennaRNA/alifold.h>
```

This variable controls the weight of the covariance term in the energy function of alignment folding algorithms.

Deprecated See [vrna_md_t.cv_fact](#), and [vrna_mfe\(\)](#) to avoid using global variables

Default is 1.

15.22.3.2 `double nc_fact`

```
#include <ViennaRNA/alifold.h>
```

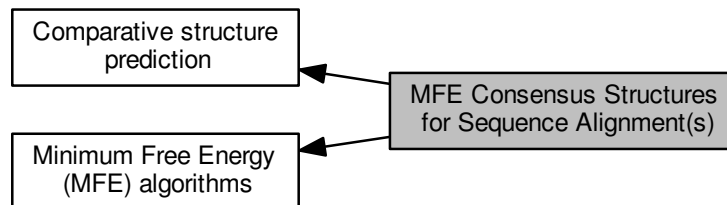
This variable controls the magnitude of the penalty for non-compatible sequences in the covariance term of alignment folding algorithms.

Deprecated See [vrna_md_t.nc_fact](#), and [vrna_mfe\(\)](#) to avoid using global variables

Default is 1.

15.23 MFE Consensus Structures for Sequence Alignment(s)

Collaboration diagram for MFE Consensus Structures for Sequence Alignment(s):



Functions

- float [vrna_alifold](#) (const char **sequences, char *structure)
Compute Minimum Free Energy (MFE), and a corresponding consensus secondary structure for an RNA sequence alignment using a comparative method.
- float [vrna_circalifold](#) (const char **sequences, char *structure)
Compute Minimum Free Energy (MFE), and a corresponding consensus secondary structure for a sequence alignment of circular RNAs using a comparative method.
- float [alifold](#) (const char **strings, char *structure)
Compute MFE and according consensus structure of an alignment of sequences.
- float [circalifold](#) (const char **strings, char *structure)
Compute MFE and according structure of an alignment of sequences assuming the sequences are circular instead of linear.
- void [free_alifold_arrays](#) (void)
Free the memory occupied by MFE alifold functions.

15.23.1 Detailed Description

15.23.2 Function Documentation

15.23.2.1 float vrna_alifold (const char ** sequences, char * structure)

```
#include <ViennaRNA/alifold.h>
```

Compute Minimum Free Energy (MFE), and a corresponding consensus secondary structure for an RNA sequence alignment using a comparative method.

This simplified interface to [vrna_mfe\(\)](#) computes the MFE and, if required, a consensus secondary structure for an RNA sequence alignment using default options. Memory required for dynamic programming (DP) matrices will be allocated and free'd on-the-fly. Hence, after return of this function, the recursively filled matrices are not available any more for any post-processing, e.g. suboptimal backtracking, etc.

Note

In case you want to use the filled DP matrices for any subsequent post-processing step, or you require other conditions than specified by the default model details, use [vrna_mfe\(\)](#), and the data structure [vrna_fold_compound_t](#) instead.

See also

[vrna_circalifold\(\)](#), [vrna_mfe\(\)](#), [vrna_fold_compound\(\)](#), [vrna_fold_compound_t](#)

Parameters

<i>sequences</i>	RNA sequence alignment
<i>structure</i>	A pointer to the character array where the secondary structure in dot-bracket notation will be written to

Returns

the minimum free energy (MFE) in kcal/mol

15.23.2.2 float vrna_circalifold (const char ** sequences, char * structure)

```
#include <ViennaRNA/alifold.h>
```

Compute Minimum Free Energy (MFE), and a corresponding consensus secondary structure for a sequence alignment of circular RNAs using a comparative method.

This simplified interface to [vrna_mfe\(\)](#) computes the MFE and, if required, a consensus secondary structure for an RNA sequence alignment using default options. Memory required for dynamic programming (DP) matrices will be allocated and free'd on-the-fly. Hence, after return of this function, the recursively filled matrices are not available any more for any post-processing, e.g. suboptimal backtracking, etc.

Folding of circular RNA sequences is handled as a post-processing step of the forward recursions. See [9] for further details.

Note

In case you want to use the filled DP matrices for any subsequent post-processing step, or you require other conditions than specified by the default model details, use [vrna_mfe\(\)](#), and the data structure [vrna_fold_compound_t](#) instead.

See also

[vrna_alifold\(\)](#), [vrna_mfe\(\)](#), [vrna_fold_compound\(\)](#), [vrna_fold_compound_t](#)

Parameters

<i>sequences</i>	Sequence alignment of circular RNAs
<i>structure</i>	A pointer to the character array where the secondary structure in dot-bracket notation will be written to

Returns

the minimum free energy (MFE) in kcal/mol

15.23.2.3 float alifold (const char ** *strings*, char * *structure*)

```
#include <ViennaRNA/alifold.h>
```

Compute MFE and according consensus structure of an alignment of sequences.

This function predicts the consensus structure for the aligned 'sequences' and returns the minimum free energy; the mfe structure in bracket notation is returned in 'structure'.

Sufficient space must be allocated for 'structure' before calling [alifold\(\)](#).

Deprecated Usage of this function is discouraged! Use [vrna_alifold\(\)](#), or [vrna_mfe\(\)](#) instead!

See also

[vrna_alifold\(\)](#), [vrna_mfe\(\)](#)

Parameters

<i>strings</i>	A pointer to a NULL terminated array of character arrays
<i>structure</i>	A pointer to a character array that may contain a constraining consensus structure (will be overwritten by a consensus structure that exhibits the MFE)

Returns

The free energy score in kcal/mol

15.23.2.4 float circalifold (const char ** *strings*, char * *structure*)

```
#include <ViennaRNA/alifold.h>
```

Compute MFE and according structure of an alignment of sequences assuming the sequences are circular instead of linear.

Deprecated Usage of this function is discouraged! Use [vrna_alicircfold\(\)](#), and [vrna_mfe\(\)](#) instead!

See also

[vrna_alicircfold\(\)](#), [vrna_alifold\(\)](#), [vrna_mfe\(\)](#)

Parameters

<i>strings</i>	A pointer to a NULL terminated array of character arrays
<i>structure</i>	A pointer to a character array that may contain a constraining consensus structure (will be overwritten by a consensus structure that exhibits the MFE)

Returns

The free energy score in kcal/mol

15.23.2.5 void free_alifold_arrays (void)

```
#include <ViennaRNA/alifold.h>
```

Free the memory occupied by MFE alifold functions.

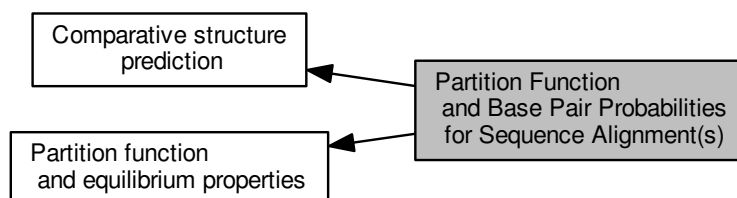
Deprecated Usage of this function is discouraged! It only affects memory being free'd that was allocated by an old API function before. Release of memory occupied by the newly introduced [vrna_fold_compound_t](#) is handled by `vrna_vrna_fold_compound_free()`

See also

`vrna_vrna_fold_compound_free()`

15.24 Partition Function and Base Pair Probabilities for Sequence Alignment(s)

Collaboration diagram for Partition Function and Base Pair Probabilities for Sequence Alignment(s):



Functions

- float [vrna_pf_alifold](#) (const char **sequences, char *structure, [vrna_plist_t](#) **pl)

Compute Partition function Q (and base pair probabilities) for an RNA sequence alignment using a comparative method.
- float [vrna_pf_circalifold](#) (const char **sequences, char *structure, [vrna_plist_t](#) **pl)

Compute Partition function Q (and base pair probabilities) for an alignment of circular RNA sequences using a comparative method.
- float [alipf_fold_par](#) (const char **sequences, char *structure, [vrna_plist_t](#) **pl, [vrna_exp_param_t](#) *parameters, int calculate_bppm, int is_constrained, int is_circular)
- float [alipf_fold](#) (const char **sequences, char *structure, [vrna_plist_t](#) **pl)

The partition function version of [alifold\(\)](#) works in analogy to [pf_fold\(\)](#). Pair probabilities and information about sequence covariations are returned via the 'pi' variable as a list of [vrna_pinfo_t](#) structs. The list is terminated by the first entry with $pi.i = 0$.
- float [alipf_circ_fold](#) (const char **sequences, char *structure, [vrna_plist_t](#) **pl)
- [FLT_OR_DBL](#) * [export_ali_bppm](#) (void)

Get a pointer to the base pair probability array.
- void [free_alipf_arrays](#) (void)

Free the memory occupied by folding matrices allocated by [alipf_fold](#), [alipf_circ_fold](#), etc.

15.24.1 Detailed Description

15.24.2 Function Documentation

15.24.2.1 float [vrna_pf_alifold](#) (const char ** sequences, char * structure, [vrna_plist_t](#) ** pl)

```
#include <ViennaRNA/alifold.h>
```

Compute Partition function Q (and base pair probabilities) for an RNA sequence alignment using a comparative method.

This simplified interface to [vrna_pf\(\)](#) computes the partition function and, if required, base pair probabilities for an RNA sequence alignment using default options. Memory required for dynamic programming (DP) matrices will be allocated and free'd on-the-fly. Hence, after return of this function, the recursively filled matrices are not available any more for any post-processing.

Note

In case you want to use the filled DP matrices for any subsequent post-processing step, or you require other conditions than specified by the default model details, use [vrna_pf\(\)](#), and the data structure [vrna_fold_compound_t](#) instead.

See also

[vrna_pf_circalifold\(\)](#), [vrna_pf\(\)](#), [vrna_fold_compound_comparative\(\)](#), [vrna_fold_compound_t](#)

Parameters

<i>sequences</i>	RNA sequence alignment
<i>structure</i>	A pointer to the character array where position-wise pairing propensity will be stored. (Maybe NULL)
<i>pl</i>	A pointer to a list of vrna_plist_t to store pairing probabilities (Maybe NULL)

Returns

The Gibbs free energy of the ensemble ($G = -RT \cdot \log(Q)$) in kcal/mol

15.24.2.2 `float vrna_pf_circalifold (const char ** sequences, char * structure, vrna_plist_t ** pl)`

```
#include <ViennaRNA/alifold.h>
```

Compute Partition function Q (and base pair probabilities) for an alignment of circular RNA sequences using a comparative method.

This simplified interface to [vrna_pf\(\)](#) computes the partition function and, if required, base pair probabilities for an RNA sequence alignment using default options. Memory required for dynamic programming (DP) matrices will be allocated and free'd on-the-fly. Hence, after return of this function, the recursively filled matrices are not available any more for any post-processing.

Note

In case you want to use the filled DP matrices for any subsequent post-processing step, or you require other conditions than specified by the default model details, use [vrna_pf\(\)](#), and the data structure [vrna_fold_compound_t](#) instead.

Folding of circular RNA sequences is handled as a post-processing step of the forward recursions. See [9] for further details.

See also

[vrna_pf_alifold\(\)](#), [vrna_pf\(\)](#), [vrna_fold_compound_comparative\(\)](#), [vrna_fold_compound_t](#)

Parameters

<i>sequences</i>	Sequence alignment of circular RNAs
<i>structure</i>	A pointer to the character array where position-wise pairing propensity will be stored. (Maybe NULL)
<i>pl</i>	A pointer to a list of vrna_plist_t to store pairing probabilities (Maybe NULL)

Returns

The Gibbs free energy of the ensemble ($G = -RT \cdot \log(Q)$) in kcal/mol

15.24.2.3 float alipf_fold_par (const char ** *sequences*, char * *structure*, vrna_plist_t ** *pl*, vrna_exp_param_t * *parameters*, int *calculate_bppm*, int *is_constrained*, int *is_circular*)

```
#include <ViennaRNA/alifold.h>
```

Deprecated Use [vrna_pf\(\)](#) instead

Parameters

<i>sequences</i>	
<i>structure</i>	
<i>pl</i>	
<i>parameters</i>	
<i>calculate_bppm</i>	
<i>is_constrained</i>	
<i>is_circular</i>	

Returns

15.24.2.4 float alipf_fold (const char ** *sequences*, char * *structure*, vrna_plist_t ** *pl*)

```
#include <ViennaRNA/alifold.h>
```

The partition function version of [alifold\(\)](#) works in analogy to [pf_fold\(\)](#). Pair probabilities and information about sequence covariations are returned via the 'pi' variable as a list of [vrna_pinfo_t](#) structs. The list is terminated by the first entry with pi.i = 0.

Deprecated Use [vrna_pf\(\)](#) instead

Parameters

<i>sequences</i>	
<i>structure</i>	
<i>pl</i>	

Returns

15.24.2.5 `float alipf_circ_fold (const char ** sequences, char * structure, vrna_plist_t ** pl)`

```
#include <ViennaRNA/alifold.h>
```

Deprecated Use [vrna_pf\(\)](#) instead

Parameters

<i>sequences</i>	
<i>structure</i>	
<i>pl</i>	

Returns

15.24.2.6 `FLT_OR_DBL* export_ali_bppm (void)`

```
#include <ViennaRNA/alifold.h>
```

Get a pointer to the base pair probability array.

Accessing the base pair probabilities for a pair (i,j) is achieved by

```
FLT_OR_DBL *pr = export_bppm(); pr_ij = pr[iindx[i]-j];
```

Deprecated Usage of this function is discouraged! The new [vrna_fold_compound_t](#) allows direct access to the folding matrices, including the pair probabilities! The pair probability array returned here reflects the one of the latest call to [vrna_pf\(\)](#), or any of the old API calls for consensus structure partition function folding.

See also

[vrna_fold_compound_t](#), [vrna_fold_compound_comparative\(\)](#), and [vrna_pf\(\)](#)

Returns

A pointer to the base pair probability array

15.24.2.7 `void free_alipf_arrays (void)`

```
#include <ViennaRNA/alifold.h>
```

Free the memory occupied by folding matrices allocated by `alipf_fold`, `alipf_circ_fold`, etc.

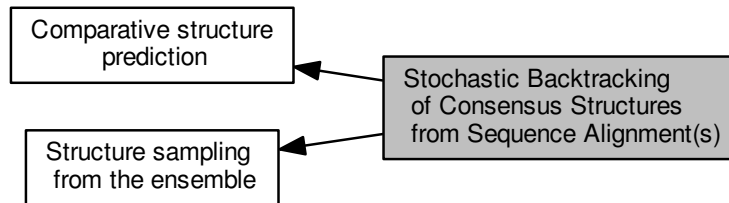
Deprecated Usage of this function is discouraged! This function only free's memory allocated by old API function calls. Memory allocated by any of the new API calls (starting with `vrna_`) will be not affected!

See also

[vrna_fold_compound_t](#), [vrna_vrna_fold_compound_free\(\)](#)

15.25 Stochastic Backtracking of Consensus Structures from Sequence Alignment(s)

Collaboration diagram for Stochastic Backtracking of Consensus Structures from Sequence Alignment(s):



Functions

- `char * alipbacktrack (double *prob)`

Sample a consensus secondary structure from the Boltzmann ensemble according its probability.

15.25.1 Detailed Description

15.25.2 Function Documentation

15.25.2.1 `char* alipbacktrack (double * prob)`

```
#include <ViennaRNA/alifold.h>
```

Sample a consensus secondary structure from the Boltzmann ensemble according its probability.

Deprecated Use `vrna_pbacktrack()` instead!

Parameters

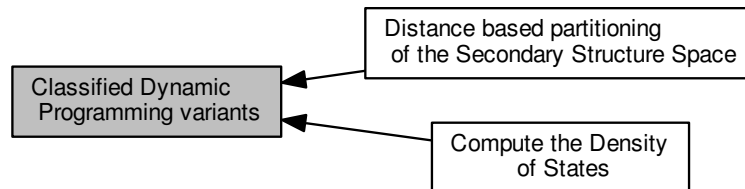
<code>prob</code>	to be described (berni)
-------------------	-------------------------

Returns

A sampled consensus secondary structure in dot-bracket notation

15.26 Classified Dynamic Programming variants

Collaboration diagram for Classified Dynamic Programming variants:



Modules

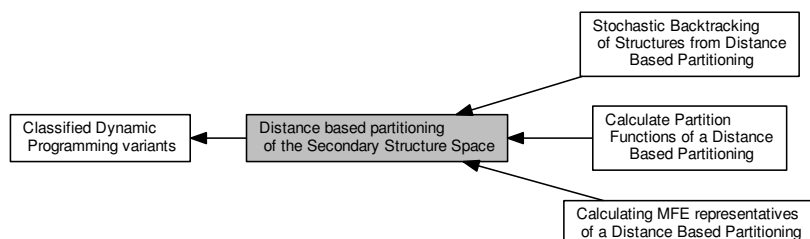
- [Distance based partitioning of the Secondary Structure Space](#)
Compute Thermodynamic properties for a Distance Class Partitioning of the Secondary Structure Space.
- [Compute the Density of States](#)

15.26.1 Detailed Description

15.27 Distance based partitioning of the Secondary Structure Space

Compute Thermodynamic properties for a Distance Class Partitioning of the Secondary Structure Space.

Collaboration diagram for Distance based partitioning of the Secondary Structure Space:



Modules

- [Calculating MFE representatives of a Distance Based Partitioning](#)
Compute the minimum free energy (MFE) and secondary structures for a partitioning of the secondary structure space according to the base pair distance to two fixed reference structures basepair distance to two fixed reference structures.
- [Calculate Partition Functions of a Distance Based Partitioning](#)
Compute the partition function and stochastically sample secondary structures for a partitioning of the secondary structure space according to the base pair distance to two fixed reference structures.
- [Stochastic Backtracking of Structures from Distance Based Partitioning](#)
Contains functions related to stochastic backtracking from a specified distance class.

Files

- file [2Dfold.h](#)
MFE structures for base pair distance classes.
- file [2Dpfold.h](#)
Partition function implementations for base pair distance classes.

15.27.1 Detailed Description

Compute Thermodynamic properties for a Distance Class Partitioning of the Secondary Structure Space.

All functions related to this group implement the basic recursions for MFE folding, partition function computation and stochastic backtracking with a *classified dynamic programming* approach. The secondary structure space is divided into partitions according to the base pair distance to two given reference structures and all relevant properties are calculated for each of the resulting partitions

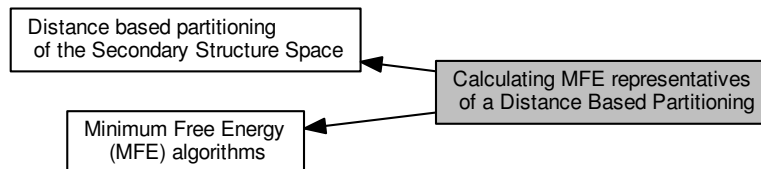
See also

For further details, we refer to Lorenz et al. 2009 [11]

15.28 Calculating MFE representatives of a Distance Based Partitioning

Compute the minimum free energy (MFE) and secondary structures for a partitioning of the secondary structure space according to the base pair distance to two fixed reference structures basepair distance to two fixed reference structures.

Collaboration diagram for Calculating MFE representatives of a Distance Based Partitioning:



Data Structures

- struct [vrna_sol_TwoD_t](#)
Solution element returned from [vrna_mfe_TwoD\(\)](#) [More...](#)
- struct [TwoDfold_vars](#)
Variables compound for 2Dfold MFE folding. [More...](#)

Typedefs

- typedef struct [vrna_sol_TwoD_t](#) [vrna_sol_TwoD_t](#)
Solution element returned from [vrna_mfe_TwoD\(\)](#)
- typedef struct [TwoDfold_vars](#) [TwoDfold_vars](#)
Variables compound for 2Dfold MFE folding.

Functions

- [vrna_sol_TwoD_t](#) * [vrna_mfe_TwoD](#) ([vrna_fold_compound_t](#) *vc, int distance1, int distance2)
Compute MFE's and representative for distance partitioning.
- char * [vrna_backtrack5_TwoD](#) ([vrna_fold_compound_t](#) *vc, int k, int l, unsigned int j)
Backtrack a minimum free energy structure from a 5' section of specified length.
- [TwoDfold_vars](#) * [get_TwoDfold_variables](#) (const char *seq, const char *structure1, const char *structure2, int circ)
Get a structure of type [TwoDfold_vars](#) prefilled with current global settings.
- void [destroy_TwoDfold_variables](#) ([TwoDfold_vars](#) *our_variables)
Destroy a [TwoDfold_vars](#) datastructure without memory loss.
- [vrna_sol_TwoD_t](#) * [TwoDfoldList](#) ([TwoDfold_vars](#) *vars, int distance1, int distance2)
Compute MFE's and representative for distance partitioning.
- char * [TwoDfold_backtrack_f5](#) (unsigned int j, int k, int l, [TwoDfold_vars](#) *vars)
Backtrack a minimum free energy structure from a 5' section of specified length.

15.28.1 Detailed Description

Compute the minimum free energy (MFE) and secondary structures for a partitioning of the secondary structure space according to the base pair distance to two fixed reference structures basepair distance to two fixed reference structures.

See also

For further details, we refer to Lorenz et al. 2009 [11]

15.28.2 Data Structure Documentation

15.28.2.1 struct vrna_sol_TwoD_t

Solution element returned from [vrna_mfe_TwoD\(\)](#)

This element contains free energy and structure for the appropriate kappa (k), lambda (l) neighborhood The data-structure contains two integer attributes 'k' and 'l' as well as an attribute 'en' of type float representing the free energy in kcal/mol and an attribute 's' of type char* containing the secondary structure representative,

A value of [INF](#) in k denotes the end of a list

See also

[vrna_mfe_TwoD\(\)](#)

Data Fields

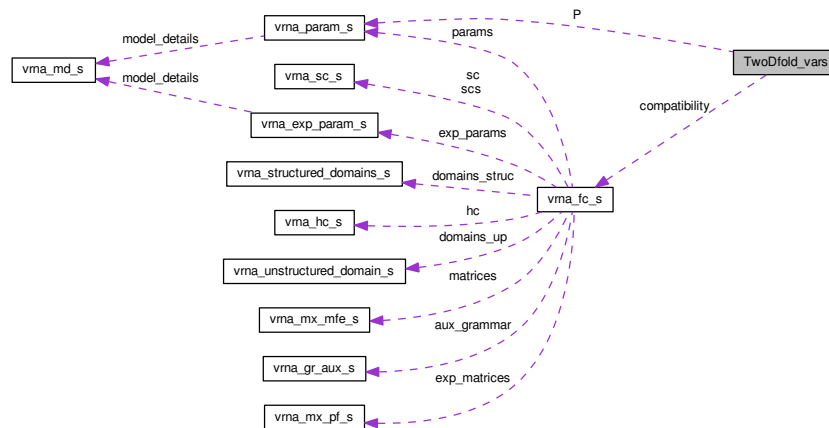
- int [k](#)
Distance to first reference.
- int [l](#)
Distance to second reference.
- float [en](#)
Free energy in kcal/mol.
- char * [s](#)
MFE representative structure in dot-bracket notation.

15.28.2.2 struct TwoDfold_vars

Variables compound for 2Dfold MFE folding.

Deprecated This data structure will be removed from the library soon! Use [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_mfe_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Collaboration diagram for TwoDfold_vars:



Data Fields

- `vrna_param_t * P`
Precomputed energy parameters and model details.
- `int do_backtrack`
Flag whether to do backtracing of the structure(s) or not.
- `char * ptype`
Precomputed array of pair types.
- `char * sequence`
The input sequence.
- `short * S1`
The input sequences in numeric form.
- `unsigned int maxD1`
Maximum allowed base pair distance to first reference.
- `unsigned int maxD2`
Maximum allowed base pair distance to second reference.
- `unsigned int * mm1`
Maximum matching matrix, reference struct 1 disallowed.
- `unsigned int * mm2`
Maximum matching matrix, reference struct 2 disallowed.
- `int * my_iindx`
Index for moving in quadratic distancey dimensions.
- `unsigned int * referenceBPs1`
Matrix containing number of basepairs of reference structure1 in interval [i,j].
- `unsigned int * referenceBPs2`
Matrix containing number of basepairs of reference structure2 in interval [i,j].
- `unsigned int * bpdist`
Matrix containing base pair distance of reference structure 1 and 2 on interval [i,j].

15.28.3 Typedef Documentation

15.28.3.1 typedef struct vrna_sol_TwoD_t vrna_sol_TwoD_t

```
#include <ViennaRNA/2Dfold.h>
```

Solution element returned from [vrna_mfe_TwoD\(\)](#)

This element contains free energy and structure for the appropriate kappa (k), lambda (l) neighborhood. The datastructure contains two integer attributes 'k' and 'l' as well as an attribute 'en' of type float representing the free energy in kcal/mol and an attribute 's' of type char* containing the secondary structure representative,

A value of [INF](#) in k denotes the end of a list

See also

[vrna_mfe_TwoD\(\)](#)

15.28.3.2 typedef struct TwoDfold_vars TwoDfold_vars

```
#include <ViennaRNA/2Dfold.h>
```

Variables compound for 2Dfold MFE folding.

Deprecated This data structure will be removed from the library soon! Use [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_mfe_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

15.28.4 Function Documentation

15.28.4.1 vrna_sol_TwoD_t* vrna_mfe_TwoD (vrna_fold_compound_t * vc, int distance1, int distance2)

```
#include <ViennaRNA/2Dfold.h>
```

Compute MFE's and representative for distance partitioning.

This function computes the minimum free energies and a representative secondary structure for each distance class according to the two references specified in the datastructure 'vars'. The maximum basepair distance to each of both references may be set by the arguments 'distance1' and 'distance2', respectively. If both distance arguments are set to '-1', no restriction is assumed and the calculation is performed for each distance class possible.

The returned list contains an entry for each distance class. If a maximum basepair distance to either of the references was passed, an entry with k=-1 will be appended in the list, denoting the class where all structures exceeding the maximum will be thrown into. The end of the list is denoted by an attribute value of [INF](#) in the k-attribute of the list entry.

See also

[vrna_fold_compound_TwoD\(\)](#), [vrna_fold_compound_free\(\)](#), [vrna_pf_TwoD\(\)](#), [vrna_backtrack5_TwoD\(\)](#), [vrna_sol_TwoD_t](#), [vrna_fold_compound_t](#)

Parameters

<i>vc</i>	The datastructure containing all precomputed folding attributes
<i>distance1</i>	maximum distance to reference1 (-1 means no restriction)
<i>distance2</i>	maximum distance to reference2 (-1 means no restriction)

Returns

A list of minimum free energies (and corresponding structures) for each distance class

15.28.4.2 `char* vrna_backtrack5_TwoD (vrna_fold_compound_t * vc, int k, int l, unsigned int j)`

```
#include <ViennaRNA/2Dfold.h>
```

Backtrack a minimum free energy structure from a 5' section of specified length.

This function allows one to backtrack a secondary structure beginning at the 5' end, a specified length and residing in a specific distance class. If the argument 'k' gets a value of -1, the structure that is backtracked is assumed to reside in the distance class where all structures exceeding the maximum basepair distance specified in [vrna_mfe_TwoD\(\)](#) belong to.

Note

The argument 'vars' must contain precalculated energy values in the energy matrices, i.e. a call to [vrna_mfe_TwoD\(\)](#) preceding this function is mandatory!

See also

[vrna_mfe_TwoD\(\)](#)

Parameters

<i>vc</i>	The datastructure containing all precomputed folding attributes
<i>j</i>	The length in nucleotides beginning from the 5' end
<i>k</i>	distance to reference1 (may be -1)
<i>l</i>	distance to reference2

15.28.4.3 `TwoDfold_vars* get_TwoDfold_variables (const char * seq, const char * structure1, const char * structure2, int circ)`

```
#include <ViennaRNA/2Dfold.h>
```

Get a structure of type [TwoDfold_vars](#) prefilled with current global settings.

This function returns a datastructure of type [TwoDfold_vars](#). The data fields inside the [TwoDfold_vars](#) are prefilled by global settings and all memory allocations necessary to start a computation are already done for the convenience of the user

Note

Make sure that the reference structures are compatible with the sequence according to Watson-Crick- and Wobble-base pairing

Deprecated Use the new API that relies on [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_mfe_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Parameters

<i>seq</i>	The RNA sequence
<i>structure1</i>	The first reference structure in dot-bracket notation
<i>structure2</i>	The second reference structure in dot-bracket notation
<i>circ</i>	A switch to indicate the assumption to fold a circular instead of linear RNA (0=OFF, 1=ON)

Returns

A datastructure prefilled with folding options and allocated memory

15.28.4.4 `void destroy_TwoDfold_variables (TwoDfold_vars * our_variables)`

```
#include <ViennaRNA/2Dfold.h>
```

Destroy a [TwoDfold_vars](#) datastructure without memory loss.

This function free's all allocated memory that depends on the datastructure given.

Deprecated Use the new API that relies on [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_mfe_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Parameters

<i>our_variables</i>	A pointer to the datastructure to be destroyed
----------------------	------------------------------------------------

15.28.4.5 `vrna_sol_TwoD_t* TwoDfoldList (TwoDfold_vars * vars, int distance1, int distance2)`

```
#include <ViennaRNA/2Dfold.h>
```

Compute MFE's and representative for distance partitioning.

This function computes the minimum free energies and a representative secondary structure for each distance class according to the two references specified in the datastructure 'vars'. The maximum basepair distance to each of both references may be set by the arguments 'distance1' and 'distance2', respectively. If both distance arguments are set to '-1', no restriction is assumed and the calculation is performed for each distance class possible.

The returned list contains an entry for each distance class. If a maximum basepair distance to either of the references was passed, an entry with $k=-1$ will be appended in the list, denoting the class where all structures exceeding the maximum will be thrown into. The end of the list is denoted by an attribute value of [INF](#) in the k -attribute of the list entry.

Deprecated Use the new API that relies on [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_mfe_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

Parameters

<i>vars</i>	the datastructure containing all predefined folding attributes
<i>distance1</i>	maximum distance to reference1 (-1 means no restriction)
<i>distance2</i>	maximum distance to reference2 (-1 means no restriction)

15.28.4.6 `char* TwoDfold_backtrack_f5 (unsigned int j, int k, int l, TwoDfold_vars * vars)`

```
#include <ViennaRNA/2Dfold.h>
```

Backtrack a minimum free energy structure from a 5' section of specified length.

This function allows one to backtrack a secondary structure beginning at the 5' end, a specified length and residing in a specific distance class. If the argument 'k' gets a value of -1, the structure that is backtracked is assumed to reside in the distance class where all structures exceeding the maximum basepair distance specified in `TwoDfold()` belong to.

Note

The argument 'vars' must contain precalculated energy values in the energy matrices, i.e. a call to `TwoDfold()` preceding this function is mandatory!

Deprecated Use the new API that relies on [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_mfe_TwoD\(\)](#), [vrna_backtrack5_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

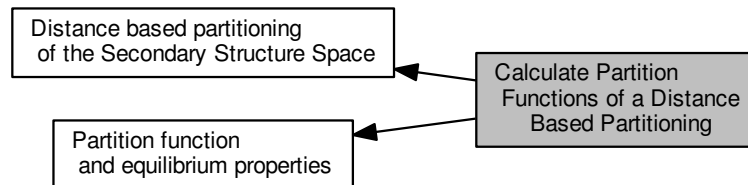
Parameters

<i>j</i>	The length in nucleotides beginning from the 5' end
<i>k</i>	distance to reference1 (may be -1)
<i>l</i>	distance to reference2
<i>vars</i>	the datastructure containing all predefined folding attributes

15.29 Calculate Partition Functions of a Distance Based Partitioning

Compute the partition function and stochastically sample secondary structures for a partitioning of the secondary structure space according to the base pair distance to two fixed reference structures.

Collaboration diagram for Calculate Partition Functions of a Distance Based Partitioning:



Data Structures

- struct [vrna_sol_TwoD_pf_t](#)
Solution element returned from [vrna_pf_TwoD\(\)](#) [More...](#)

Typedefs

- typedef struct [vrna_sol_TwoD_pf_t](#) [vrna_sol_TwoD_pf_t](#)
Solution element returned from [vrna_pf_TwoD\(\)](#)

Functions

- [vrna_sol_TwoD_pf_t](#) * [vrna_pf_TwoD](#) ([vrna_fold_compound_t](#) *vc, int maxDistance1, int maxDistance2)
Compute the partition function for all distance classes.

15.29.1 Detailed Description

Compute the partition function and stochastically sample secondary structures for a partitioning of the secondary structure space according to the base pair distance to two fixed reference structures.

15.29.2 Data Structure Documentation

15.29.2.1 struct [vrna_sol_TwoD_pf_t](#)

Solution element returned from [vrna_pf_TwoD\(\)](#)

This element contains the partition function for the appropriate kappa (k), lambda (l) neighborhood. The datastructure contains two integer attributes 'k' and 'l' as well as an attribute 'q' of type [FLT_OR_DBL](#).

A value of [INF](#) in k denotes the end of a list.

See also

[vrna_pf_TwoD\(\)](#)

Data Fields

- `int k`
Distance to first reference.
- `int l`
Distance to second reference.
- `FLT_OR_DBL q`
partition function

15.29.3 Typedef Documentation

15.29.3.1 `typedef struct vrna_sol_TwoD_pf_t vrna_sol_TwoD_pf_t`

```
#include <ViennaRNA/2Dpfold.h>
```

Solution element returned from `vrna_pf_TwoD()`

This element contains the partition function for the appropriate kappa (k), lambda (l) neighborhood. The datastructure contains two integer attributes 'k' and 'l' as well as an attribute 'q' of type `FLT_OR_DBL`.

A value of `INF` in k denotes the end of a list.

See also

`vrna_pf_TwoD()`

15.29.4 Function Documentation

15.29.4.1 `vrna_sol_TwoD_pf_t* vrna_pf_TwoD(vrna_fold_compound_t* vc, int maxDistance1, int maxDistance2)`

```
#include <ViennaRNA/2Dpfold.h>
```

Compute the partition function for all distance classes.

This function computes the partition functions for all distance classes according to the two reference structures specified in the datastructure 'vars'. Similar to `vrna_mfe_TwoD()` the arguments `maxDistance1` and `maxDistance2` specify the maximum distance to both reference structures. A value of '-1' in either of them makes the appropriate distance restrictionless, i.e. all basepair distances to the reference are taken into account during computation. In case there is a restriction, the returned solution contains an entry where the attribute `k=l=-1` contains the partition function for all structures exceeding the restriction. A value of `INF` in the attribute 'k' of the returned list denotes the end of the list.

See also

`vrna_fold_compound_TwoD()`, `vrna_fold_compound_free()`, `vrna_fold_compound`, `vrna_sol_TwoD_pf_t`

Parameters

<code>vc</code>	The datastructure containing all necessary folding attributes and matrices
<code>maxDistance1</code>	The maximum basepair distance to reference1 (may be -1)
<code>maxDistance2</code>	The maximum basepair distance to reference2 (may be -1)

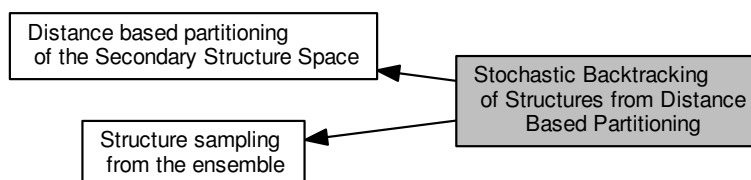
Returns

A list of partition funtions for the corresponding distance classes

15.30 Stochastic Backtracking of Structures from Distance Based Partitioning

Contains functions related to stochastic backtracking from a specified distance class.

Collaboration diagram for Stochastic Backtracking of Structures from Distance Based Partitioning:



Functions

- `char * vrna_pbacktrack_TwoD (vrna_fold_compound_t *vc, int d1, int d2)`
Sample secondary structure representatives from a set of distance classes according to their Boltzmann probability.
- `char * vrna_pbacktrack5_TwoD (vrna_fold_compound_t *vc, int d1, int d2, unsigned int length)`
Sample secondary structure representatives with a specified length from a set of distance classes according to their Boltzmann probability.

15.30.1 Detailed Description

Contains functions related to stochastic backtracking from a specified distance class.

15.30.2 Function Documentation

15.30.2.1 `char* vrna_pbacktrack_TwoD (vrna_fold_compound_t * vc, int d1, int d2)`

```
#include <ViennaRNA/2Dpfold.h>
```

Sample secondary structure representatives from a set of distance classes according to their Boltzmann probability.

If the argument 'd1' is set to '-1', the structure will be backtracked in the distance class where all structures exceeding the maximum basepair distance to either of the references reside.

Precondition

The argument 'vars' must contain precalculated partition function matrices, i.e. a call to `vrna_pf_TwoD()` preceding this function is mandatory!

See also

[vrna_pf_TwoD\(\)](#)

Parameters

<code>in, out</code>	<code>vc</code>	The vrna_fold_compound_t datastructure containing all necessary folding attributes and matrices
<code>in</code>	<code>d1</code>	The distance to reference1 (may be -1)
<code>in</code>	<code>d2</code>	The distance to reference2

Returns

A sampled secondary structure in dot-bracket notation

15.30.2.2 `char* vrna_pbacktrack5_TwoD (vrna_fold_compound_t * vc, int d1, int d2, unsigned int length)`

```
#include <ViennaRNA/2Dpfold.h>
```

Sample secondary structure representatives with a specified length from a set of distance classes according to their Boltzmann probability.

This function does essentially the same as [vrna_pbacktrack_TwoD\(\)](#) with the only difference that partial structures, i.e. structures beginning from the 5' end with a specified length of the sequence, are backtracked

Note

This function does not work (since it makes no sense) for circular RNA sequences!

Precondition

The argument 'vars' must contain precalculated partition function matrices, i.e. a call to [vrna_pf_TwoD\(\)](#) preceding this function is mandatory!

See also

[vrna_pbacktrack_TwoD\(\)](#), [vrna_pf_TwoD\(\)](#)

Parameters

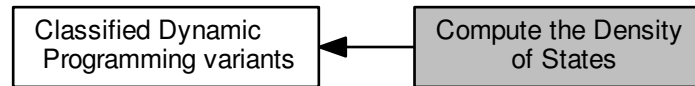
<code>in, out</code>	<code>vc</code>	The vrna_fold_compound_t datastructure containing all necessary folding attributes and matrices
<code>in</code>	<code>d1</code>	The distance to reference1 (may be -1)
<code>in</code>	<code>d2</code>	The distance to reference2
<code>in</code>	<code>length</code>	The length of the structure beginning from the 5' end

Returns

A sampled secondary structure in dot-bracket notation

15.31 Compute the Density of States

Collaboration diagram for Compute the Density of States:



Variables

- int [density_of_states](#) [MAXDOS+1]

The Density of States.

15.31.1 Detailed Description

15.31.2 Variable Documentation

15.31.2.1 int density_of_states[MAXDOS+1]

```
#include <ViennaRNA/subopt.h>
```

The Density of States.

This array contains the density of states for an RNA sequences after a call to [subopt_par\(\)](#), [subopt\(\)](#) or [subopt_circ\(\)](#).

Precondition

Call one of the functions [subopt_par\(\)](#), [subopt\(\)](#) or [subopt_circ\(\)](#) prior accessing the contents of this array

See also

[subopt_par\(\)](#), [subopt\(\)](#), [subopt_circ\(\)](#)

15.32 Inverse Folding (Design)

RNA sequence design.

Files

- file [inverse.h](#)
Inverse folding routines.

Functions

- float [inverse_fold](#) (char *start, const char *target)
Find sequences with predefined structure.
- float [inverse_pf_fold](#) (char *start, const char *target)
Find sequence that maximizes probability of a predefined structure.

Variables

- char * [symbolset](#)
This global variable points to the allowed bases, initially "AUGC". It can be used to design sequences from reduced alphabets.
- float [final_cost](#)
- int [give_up](#)
- int [inv_verbose](#)

15.32.1 Detailed Description

RNA sequence design.

15.32.2 Function Documentation

15.32.2.1 float [inverse_fold](#) (char * *start*, const char * *target*)

```
#include <ViennaRNA/inverse.h>
```

Find sequences with predefined structure.

This function searches for a sequence with minimum free energy structure provided in the parameter 'target', starting with sequence 'start'. It returns 0 if the search was successful, otherwise a structure distance in terms of the energy difference between the search result and the actual target 'target' is returned. The found sequence is returned in 'start'. If [give_up](#) is set to 1, the function will return as soon as it is clear that the search will be unsuccessful, this speeds up the algorithm if you are only interested in exact solutions.

Parameters

<i>start</i>	The start sequence
<i>target</i>	The target secondary structure in dot-bracket notation

Returns

The distance to the target in case a search was unsuccessful, 0 otherwise

15.32.2.2 float inverse_pf_fold (char * *start*, const char * *target*)

```
#include <ViennaRNA/inverse.h>
```

Find sequence that maximizes probability of a predefined structure.

This function searches for a sequence with maximum probability to fold into the provided structure 'target' using the partition function algorithm. It returns $-kT \cdot \log(p)$ where p is the frequency of 'target' in the ensemble of possible structures. This is usually much slower than [inverse_fold\(\)](#).

Parameters

<i>start</i>	The start sequence
<i>target</i>	The target secondary structure in dot-bracket notation

Returns

The distance to the target in case a search was unsuccessful, 0 otherwise

15.32.3 Variable Documentation**15.32.3.1 float final_cost**

```
#include <ViennaRNA/inverse.h>
```

when to stop [inverse_pf_fold\(\)](#)

15.32.3.2 int give_up

```
#include <ViennaRNA/inverse.h>
```

default 0: try to minimize structure distance even if no exact solution can be found

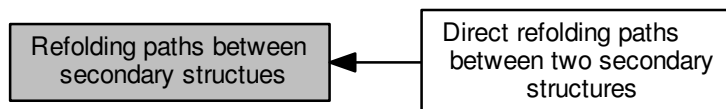
15.32.3.3 int inv_verbose

```
#include <ViennaRNA/inverse.h>
```

print out substructure on which [inverse_fold\(\)](#) fails

15.33 Refolding paths between secondary structures

Collaboration diagram for Refolding paths between secondary structures:



Modules

- [Direct refolding paths between two secondary structures](#)

Heuristics to explore direct, optimal (re-)folding paths between two secondary structures.

Files

- file [findpath.h](#)

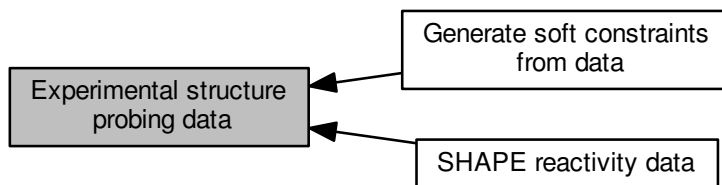
A breadth-first search heuristic for optimal direct folding paths.

15.33.1 Detailed Description

15.34 Experimental structure probing data

Include experimental structure probing data to guide structure predictions.

Collaboration diagram for Experimental structure probing data:



Modules

- [SHAPE reactivity data](#)

Incorporate SHAPE reactivity structure probing data into the folding recursions by means of soft constraints.

- [Generate soft constraints from data](#)

Find a vector of perturbation energies that minimizes the discrepancies between predicted and observed pairing probabilities and the amount of necessary adjustments.

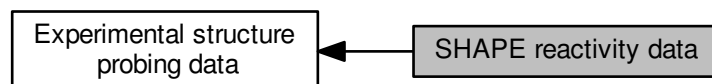
15.34.1 Detailed Description

Include experimental structure probing data to guide structure predictions.

15.35 SHAPE reactivity data

Incorporate SHAPE reactivity structure probing data into the folding recursions by means of soft constraints.

Collaboration diagram for SHAPE reactivity data:



Files

- file [constraints_SHAPE.h](#)

This module provides function to incorporate SHAPE reactivity data into the folding recursions by means of soft constraints.

Functions

- int [vrna_sc_add_SHAPE_deigan](#) ([vrna_fold_compound_t](#) *vc, const double *reactivities, double m, double b, unsigned int options)
Add SHAPE reactivity data as soft constraints (Deigan et al. method)
- int [vrna_sc_add_SHAPE_deigan_al](#)i ([vrna_fold_compound_t](#) *vc, const char **shape_files, const int *shape_file_association, double m, double b, unsigned int options)
Add SHAPE reactivity data from files as soft constraints for consensus structure prediction (Deigan et al. method)
- int [vrna_sc_add_SHAPE_zarringhalam](#) ([vrna_fold_compound_t](#) *vc, const double *reactivities, double b, double default_value, const char *shape_conversion, unsigned int options)
Add SHAPE reactivity data as soft constraints (Zarringhalam et al. method)
- int [vrna_sc_SHAPE_to_pr](#) (const char *shape_conversion, double *values, int length, double default_value)
Convert SHAPE reactivity values to probabilities for being unpaired.

15.35.1 Detailed Description

Incorporate SHAPE reactivity structure probing data into the folding recursions by means of soft constraints.

Details for our implementation to incorporate SHAPE reactivity data to guide secondary structure prediction can be found in [13]

15.35.2 Function Documentation

15.35.2.1 `int vrna_sc_add_SHAPE_deigan (vrna_fold_compound_t * vc, const double * reactivities, double m, double b, unsigned int options)`

```
#include <ViennaRNA/constraints_SHAPE.h>
```

Add SHAPE reactivity data as soft constraints (Deigan et al. method)

This approach of SHAPE directed RNA folding uses the simple linear ansatz

$$\Delta G_{\text{SHAPE}}(i) = m \ln(\text{SHAPE reactivity}(i) + 1) + b$$

to convert SHAPE reactivity values to pseudo energies whenever a nucleotide i contributes to a stacked pair. A positive slope m penalizes high reactivities in paired regions, while a negative intercept b results in a confirmatory "bonus" free energy for correctly predicted base pairs. Since the energy evaluation of a base pair stack involves two pairs, the pseudo energies are added for all four contributing nucleotides. Consequently, the energy term is applied twice for pairs inside a helix and only once for pairs adjacent to other structures. For all other loop types the energy model remains unchanged even when the experimental data highly disagrees with a certain motif.

See also

For further details, we refer to [4].

[vrna_sc_remove\(\)](#), [vrna_sc_add_SHAPE_zarringhalam\(\)](#), [vrna_sc_minimize_perturbation\(\)](#)

Parameters

<i>vc</i>	The vrna_fold_compound_t the soft constraints are associated with
<i>reactivities</i>	A vector of normalized SHAPE reactivities
<i>m</i>	The slope of the conversion function
<i>b</i>	The intercept of the conversion function
<i>options</i>	The options flag indicating how/where to store the soft constraints

Returns

1 on successful extraction of the method, 0 on errors

SWIG Wrapper Notes This function is attached as method `sc_add_SHAPE_deigan()` to objects of type `fold_compound`

15.35.2.2 `int vrna_sc_add_SHAPE_deigan_aln (vrna_fold_compound_t * vc, const char ** shape_files, const int * shape_file_association, double m, double b, unsigned int options)`

```
#include <ViennaRNA/constraints_SHAPE.h>
```

Add SHAPE reactivity data from files as soft constraints for consensus structure prediction (Deigan et al. method)

Parameters

<i>vc</i>	The vrna_fold_compound_t the soft constraints are associated with
<i>shape_files</i>	A set of filenames that contain normalized SHAPE reactivity data
<i>shape_file_association</i>	An array of integers that associate the files with sequences in the alignment
<i>m</i>	The slope of the conversion function
<i>b</i>	The intercept of the conversion function
<i>options</i>	The options flag indicating how/where to store the soft constraints

Returns

1 on successful extraction of the method, 0 on errors

SWIG Wrapper Notes This function is attached as method `sc_add_SHAPE_deigan_ali()` to objects of type `fold_compound`

15.35.2.3 `int vrna_sc_add_SHAPE_zarringhalam (vrna_fold_compound_t * vc, const double * reactivities, double b, double default_value, const char * shape_conversion, unsigned int options)`

```
#include <ViennaRNA/constraints_SHAPE.h>
```

Add SHAPE reactivity data as soft constraints (Zarringhalam et al. method)

This method first converts the observed SHAPE reactivity of nucleotide i into a probability q_i that position i is unpaired by means of a non-linear map. Then pseudo-energies of the form

$$\Delta G_{\text{SHAPE}}(x, i) = \beta |x_i - q_i|$$

are computed, where $x_i = 0$ if position i is unpaired and $x_i = 1$ if i is paired in a given secondary structure. The parameter β serves as scaling factor. The magnitude of discrepancy between prediction and experimental observation is represented by $|x_i - q_i|$.

See also

For further details, we refer to [22]

`vrna_sc_remove()`, `vrna_sc_add_SHAPE_deigan()`, `vrna_sc_minimize_pertubation()`

Parameters

<code>vc</code>	The <code>vrna_fold_compound_t</code> the soft constraints are associated with
<code>reactivities</code>	A vector of normalized SHAPE reactivities
<code>b</code>	The scaling factor β of the conversion function
<code>default_value</code>	The default value for a nucleotide where reactivity data is missing for
<code>shape_conversion</code>	A flag that specifies how to convert reactivities to probabilities
<code>options</code>	The options flag indicating how/where to store the soft constraints

Returns

1 on successful extraction of the method, 0 on errors

SWIG Wrapper Notes This function is attached as method `sc_add_SHAPE_zarringhalam()` to objects of type `fold_compound`

15.35.2.4 `int vrna_sc_SHAPE_to_pr (const char * shape_conversion, double * values, int length, double default_value)`

```
#include <ViennaRNA/constraints_SHAPE.h>
```

Convert SHAPE reactivity values to probabilities for being unpaired.

This function parses the informations from a given file and stores the result in the preallocated string sequence and the `FLT_OR_DBL` array values.

See also

[vrna_file_SHAPE_read\(\)](#)

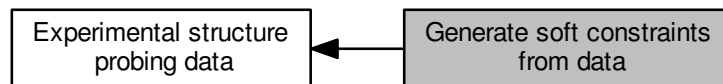
Parameters

<i>shape_conversion</i>	String defining the method used for the conversion process
<i>values</i>	Pointer to an array of SHAPE reactivities
<i>length</i>	Length of the array of SHAPE reactivities
<i>default_value</i>	Result used for position with invalid/missing reactivity values

15.36 Generate soft constraints from data

Find a vector of perturbation energies that minimizes the discrepancies between predicted and observed pairing probabilities and the amount of necessary adjustments.

Collaboration diagram for Generate soft constraints from data:



Files

- file [perturbation_fold.h](#)

Find a vector of perturbation energies that minimizes the discrepancies between predicted and observed pairing probabilities and the amount of necessary adjustments.

Macros

- `#define VRNA_OBJECTIVE_FUNCTION_QUADRATIC 0`
Use the sum of squared aberrations as objective function.
- `#define VRNA_OBJECTIVE_FUNCTION_ABSOLUTE 1`
Use the sum of absolute aberrations as objective function.
- `#define VRNA_MINIMIZER_DEFAULT 0`
Use a custom implementation of the gradient descent algorithm to minimize the objective function.
- `#define VRNA_MINIMIZER_CONJUGATE_FR 1`
Use the GNU Scientific Library implementation of the Fletcher-Reeves conjugate gradient algorithm to minimize the objective function.
- `#define VRNA_MINIMIZER_CONJUGATE_PR 2`
Use the GNU Scientific Library implementation of the Polak-Ribiere conjugate gradient algorithm to minimize the objective function.
- `#define VRNA_MINIMIZER_VECTOR_BFGS 3`
Use the GNU Scientific Library implementation of the vector Broyden-Fletcher-Goldfarb-Shanno algorithm to minimize the objective function.
- `#define VRNA_MINIMIZER_VECTOR_BFGS2 4`
Use the GNU Scientific Library implementation of the vector Broyden-Fletcher-Goldfarb-Shanno algorithm to minimize the objective function.
- `#define VRNA_MINIMIZER_STEEPEST_DESCENT 5`
Use the GNU Scientific Library implementation of the steepest descent algorithm to minimize the objective function.

Typedefs

- `typedef void(* progress_callback) (int iteration, double score, double *epsilon)`
Callback for following the progress of the minimization process.

Functions

- void `vrna_sc_minimize_perturbation` (`vrna_fold_compound_t` *vc, const double *q_prob_unpaired, int objective_function, double sigma_squared, double tau_squared, int algorithm, int sample_size, double *epsilon, double initialStepSize, double minStepSize, double minImprovement, double minimizerTolerance, `progress_callback` callback)

Find a vector of perturbation energies that minimizes the discrepancies between predicted and observed pairing probabilities and the amount of necessary adjustments.

15.36.1 Detailed Description

Find a vector of perturbation energies that minimizes the discrepancies between predicted and observed pairing probabilities and the amount of necessary adjustments.

15.36.2 Macro Definition Documentation

15.36.2.1 `#define VRNA_OBJECTIVE_FUNCTION_QUADRATIC 0`

```
#include <ViennaRNA/perturbation_fold.h>
```

Use the sum of squared aberrations as objective function.

$$F(\vec{\epsilon}) = \sum_{i=1}^n \frac{\epsilon_i^2}{\tau^2} + \sum_{i=1}^n \frac{(p_i(\vec{\epsilon}) - q_i)^2}{\sigma^2} \rightarrow \min$$

15.36.2.2 `#define VRNA_OBJECTIVE_FUNCTION_ABSOLUTE 1`

```
#include <ViennaRNA/perturbation_fold.h>
```

Use the sum of absolute aberrations as objective function.

$$F(\vec{\epsilon}) = \sum_{i=1}^n \frac{|\epsilon_i|}{\tau^2} + \sum_{i=1}^n \frac{|p_i(\vec{\epsilon}) - q_i|}{\sigma^2} \rightarrow \min$$

15.36.2.3 `#define VRNA_MINIMIZER_CONJUGATE_FR 1`

```
#include <ViennaRNA/perturbation_fold.h>
```

Use the GNU Scientific Library implementation of the Fletcher-Reeves conjugate gradient algorithm to minimize the objective function.

Please note that this algorithm can only be used when the GNU Scientific Library is available on your system

15.36.2.4 `#define VRNA_MINIMIZER_CONJUGATE_PR 2`

```
#include <ViennaRNA/perturbation_fold.h>
```

Use the GNU Scientific Library implementation of the Polak-Ribiere conjugate gradient algorithm to minimize the objective function.

Please note that this algorithm can only be used when the GNU Scientific Library is available on your system

15.36.2.5 `#define VRNA_MINIMIZER_VECTOR_BFGS 3`

```
#include <ViennaRNA/perturbation_fold.h>
```

Use the GNU Scientific Library implementation of the vector Broyden-Fletcher-Goldfarb-Shanno algorithm to minimize the objective function.

Please note that this algorithm can only be used when the GNU Scientific Library is available on your system

15.36.2.6 `#define VRNA_MINIMIZER_VECTOR_BFGS2 4`

```
#include <ViennaRNA/perturbation_fold.h>
```

Use the GNU Scientific Library implementation of the vector Broyden-Fletcher-Goldfarb-Shanno algorithm to minimize the objective function.

Please note that this algorithm can only be used when the GNU Scientific Library is available on your system

15.36.2.7 `#define VRNA_MINIMIZER_STEEPEST_DESCENT 5`

```
#include <ViennaRNA/perturbation_fold.h>
```

Use the GNU Scientific Library implementation of the steepest descent algorithm to minimize the objective function.

Please note that this algorithm can only be used when the GNU Scientific Library is available on your system

15.36.3 Typedef Documentation

15.36.3.1 `typedef void(* progress_callback)(int iteration, double score, double *epsilon)`

```
#include <ViennaRNA/perturbation_fold.h>
```

Callback for following the progress of the minimization process.

Parameters

<i>iteration</i>	The number of the current iteration
<i>score</i>	The score of the objective function
<i>epsilon</i>	The perturbation vector yielding the reported score

15.36.4 Function Documentation

15.36.4.1 `void vrna_sc_minimize_perturbation (vrna_fold_compound_t * vc, const double * q_prob_unpaired, int objective_function, double sigma_squared, double tau_squared, int algorithm, int sample_size, double * epsilon, double initialStepSize, double minStepSize, double minImprovement, double minimizerTolerance, progress_callback callback)`

```
#include <ViennaRNA/perturbation_fold.h>
```

Find a vector of perturbation energies that minimizes the discrepancies between predicted and observed pairing probabilities and the amount of necessary adjustments.

Use an iterative minimization algorithm to find a vector of perturbation energies whose incorporation as soft constraints shifts the predicted pairing probabilities closer to the experimentally observed probabilities. The algorithm aims to minimize an objective function that penalizes discrepancies between predicted and observed pairing probabilities and energy model adjustments, i.e. an appropriate vector of perturbation energies satisfies

$$F(\vec{\epsilon}) = \sum_{\mu} \frac{\epsilon_{\mu}^2}{\tau^2} + \sum_{i=1}^n \frac{(p_i(\vec{\epsilon}) - q_i)^2}{\sigma^2} \rightarrow \min.$$

An initialized fold compound and an array containing the observed probability for each nucleotide to be unbound are required as input data. The parameters `objective_function`, `sigma_squared` and `tau_squared` are responsible for adjusting the aim of the objective function. Dependend on which type of objective function is selected, either squared or absolute aberrations are contributing to the objective function. The ratio of the parameters `sigma_squared` and `tau_squared` can be used to adjust the algorithm to find a solution either close to the thermodynamic prediction (`sigma_squared` >> `tau_squared`) or close to the experimental data (`tau_squared` >> `sigma_squared`). The minimization can be performed by making use of a custom gradient descent implementation or using one of the minimizing algorithms provided by the GNU Scientific Library. All algorithms require the evaluation of the gradient of the objective function, which includes the evaluation of conditional pairing probabilities. Since an exact evaluation is expensive, the probabilities can also be estimated from sampling by setting an appropriate sample size. The found vector of perturbation energies will be stored in the array `epsilon`. The progress of the minimization process can be tracked by implementing and passing a callback function.

See also

For further details we refere to [20].

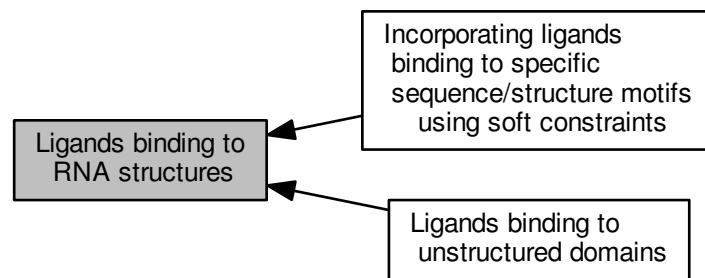
Parameters

<code>vc</code>	Pointer to a fold compound
<code>q_prob_unpaired</code>	Pointer to an array containing the probability to be unpaired for each nucleotide
<code>objective_function</code>	The type of objective function to be used (VRNA_OBJECTIVE_FUNCTION_QUADRATIC / VRNA_OBJECTIVE_FUNCTION_LINEAR)
<code>sigma_squared</code>	A factor used for weighting the objective function. More weight on this factor will lead to a solution close to the null vector.
<code>tau_squared</code>	A factor used for weighting the objective function. More weight on this factor will lead to a solution close to the data provided in <code>q_prob_unpaired</code> .
<code>algorithm</code>	The minimization algorithm (VRNA_MINIMIZER_*)
<code>sample_size</code>	The number of sampled sequences used for estimating the pairing probabilities. A value <= 0 will lead to an exact evaluation.
<code>epsilon</code>	A pointer to an array used for storing the calculated vector of perturbation energies
<code>callback</code>	A pointer to a callback function used for reporting the current minimization progress

15.37 Ligands binding to RNA structures

Simple extensions to model ligand binding to RNA structures.

Collaboration diagram for Ligands binding to RNA structures:



Modules

- [Ligands binding to unstructured domains](#)
Add ligand binding to loop regions using the [Unstructured domains](#) feature.
- [Incorporating ligands binding to specific sequence/structure motifs using soft constraints](#)
Ligand binding to specific hairpin/interior loop like motifs using the [Soft constraints](#) feature.

Files

- file [constraints_ligand.h](#)
Functions for incorporation of ligands binding to hairpin and interior loop motifs using the soft constraints framework.

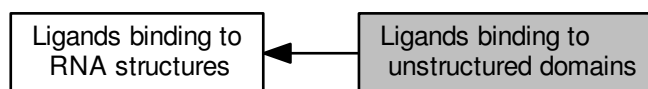
15.37.1 Detailed Description

Simple extensions to model ligand binding to RNA structures.

15.38 Ligands binding to unstructured domains

Add ligand binding to loop regions using the [Unstructured domains](#) feature.

Collaboration diagram for Ligands binding to unstructured domains:



Add ligand binding to loop regions using the [Unstructured domains](#) feature.

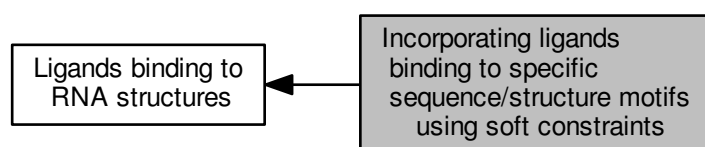
Sometime, certain ligands, like single strand binding (SSB) proteins, compete with intramolecular base pairing of the RNA. In situations, where the dissociation constant of the ligand is known and the ligand binds to a consecutive stretch of single-stranded nucleotides we can use the [Unstructured domains](#) functionality to extend the RNA folding grammar. This module provides a convenience default implementation that covers most of the application scenarios.

The function `vrna_ud_add_motif()` attaches a ligands sequence motif and corresponding binding free energy to the list of known ligand motifs within a `vrna_fold_compound_t.domains_up` attribute. The first call to this function initializes the [Unstructured domains](#) feature with our default implementation. Subsequent calls of secondary structure prediction algorithms with the modified `vrna_fold_compound_t` then directly include the competition of the ligand with regulas base pairing. Since we utilize the unstructured domain extension, The ligand binding model can be removed again using the `vrna_ud_remove()` function.

15.39 Incorporating ligands binding to specific sequence/structure motifs using soft constraints

Ligand binding to specific hairpin/interior loop like motifs using the [Soft constraints](#) feature.

Collaboration diagram for Incorporating ligands binding to specific sequence/structure motifs using soft constraints:



Functions

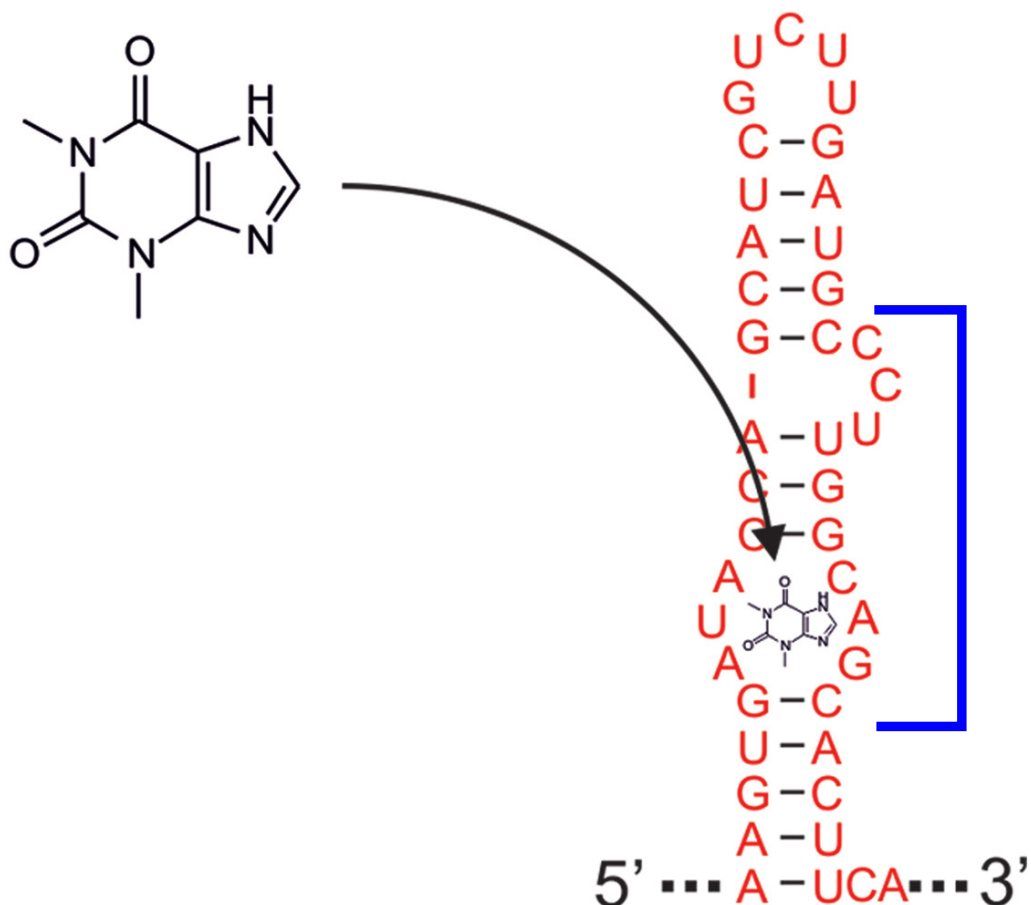
- int [vrna_sc_add_hi_motif](#) ([vrna_fold_compound_t](#) *vc, const char *seq, const char *structure, [FLT_OR_DBL](#) energy, unsigned int options)

Add soft constraints for hairpin or interior loop binding motif.

15.39.1 Detailed Description

Ligand binding to specific hairpin/interior loop like motifs using the [Soft constraints](#) feature.

Here is an example that adds a theophylline binding motif. Free energy contribution is derived from $k_d = 0.32 \mu\text{mol/l}$, taken from Jenison et al. 1994



```
vrna_sc_add_hi_motif( vc,
    "GAUACCAG&CCCUUGGCAGC",
    "...((((&)...))...)",
    -9.22, VRNA_OPTION_DEFAULT);
```

15.39.2 Function Documentation

15.39.2.1 int vrna_sc_add_hi_motif (vrna_fold_compound_t * vc, const char * seq, const char * structure, FLT_OR_DBL energy, unsigned int options)

```
#include <ViennaRNA/constraints_ligand.h>
```

Add soft constraints for hairpin or interior loop binding motif.

Parameters

<i>vc</i>	The vrna_fold_compound_t the motif is applied to
<i>seq</i>	The sequence motif (may be interspaced by '&' character)
<i>structure</i>	The structure motif (may be interspaced by '&' character)
<i>energy</i>	The free energy of the motif (e.g. binding free energy)
<i>options</i>	Options

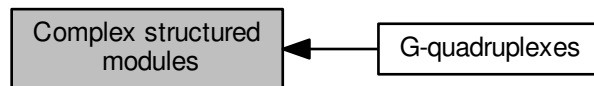
Returns

non-zero value if application of the motif using soft constraints was successful

SWIG Wrapper Notes This function is attached as method **sc_add_hi_motif()** to objects of type *fold_compound*

15.40 Complex structured modules

Collaboration diagram for Complex structured modules:



Modules

- [G-quadruplexes](#)
Various functions related to G-quadruplex computations.

Files

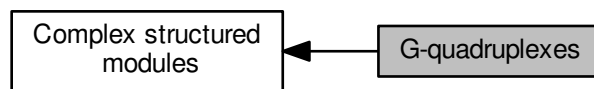
- file [gquad.h](#)
G-quadruplexes.

15.40.1 Detailed Description

15.41 G-quadruplexes

Various functions related to G-quadruplex computations.

Collaboration diagram for G-quadruplexes:



Functions

- `int * get_gquad_matrix (short *S, vrna_param_t *P)`
Get a triangular matrix prefilled with minimum free energy contributions of G-quadruplexes.
- `int parse_gquad (const char *struc, int *L, int l[3])`
- `PRIVATE int backtrack_GQuad_IntLoop (int c, int i, int j, int type, short *S, int *ggg, int *index, int *p, int *q, vrna_param_t *P)`
- `PRIVATE int backtrack_GQuad_IntLoop_L (int c, int i, int j, int type, short *S, int **ggg, int maxdist, int *p, int *q, vrna_param_t *P)`

15.41.1 Detailed Description

Various functions related to G-quadruplex computations.

15.41.2 Function Documentation

15.41.2.1 `int* get_gquad_matrix (short * S, vrna_param_t * P)`

```
#include <ViennaRNA/gquad.h>
```

Get a triangular matrix prefilled with minimum free energy contributions of G-quadruplexes.

At each position *ij* in the matrix, the minimum free energy of any G-quadruplex delimited by *i* and *j* is stored. If no G-quadruplex formation is possible, the matrix element is set to INF. Access the elements in the matrix via `matrix[indx[j]+i]`. To get the integer array `indx` see `get_jindx()`.

See also

`get_jindx()`, `encode_sequence()`

Parameters

<i>S</i>	The encoded sequence
<i>P</i>	A pointer to the data structure containing the precomputed energy contributions

Returns

A pointer to the G-quadruplex contribution matrix

15.41.2.2 `int parse_gquad (const char * struc, int * L, int l[3])`

```
#include <ViennaRNA/gquad.h>
```

given a dot-bracket structure (possibly) containing gquads encoded by '+' signs, find first gquad, return end position or 0 if none found Upon return *L* and *l[]* contain the number of stacked layers, as well as the lengths of the linker regions. To parse a string with many gquads, call `parse_gquad` repeatedly e.g. `end1 = parse_gquad(struc, &L, l); ... ; end2 = parse_gquad(struc+end1, &L, l); end2+=end1; ... ; end3 = parse_gquad(struc+end2, &L, l); end3+=end2; ... ;`

15.41.2.3 `PRIVATE int backtrack_GQuad_IntLoop (int c, int i, int j, int type, short * S, int * ggg, int * index, int * p, int * q, vrna_param_t * P)`

```
#include <ViennaRNA/gquad.h>
```

backtrack an interior loop like enclosed g-quadruplex with closing pair (i,j)

Parameters

<i>c</i>	The total contribution the loop should resemble
<i>i</i>	position i of enclosing pair
<i>j</i>	position j of enclosing pair
<i>type</i>	base pair type of enclosing pair (must be reverse type)
<i>S</i>	integer encoded sequence
<i>ggg</i>	triangular matrix containing g-quadruplex contributions
<i>index</i>	the index for accessing the triangular matrix
<i>p</i>	here the 5' position of the gquad is stored
<i>q</i>	here the 3' position of the gquad is stored
<i>P</i>	the datastructure containing the precalculated contributions

Returns

1 on success, 0 if no gquad found

15.41.2.4 `PRIVATE int backtrack_GQuad_IntLoop_L (int c, int i, int j, int type, short * S, int ** ggg, int maxdist, int * p, int * q, vrna_param_t * P)`

```
#include <ViennaRNA/gquad.h>
```

backtrack an interior loop like enclosed g-quadruplex with closing pair (i,j) with underlying Lfold matrix

Parameters

<i>c</i>	The total contribution the loop should resemble
<i>i</i>	position i of enclosing pair
<i>j</i>	position j of enclosing pair
<i>type</i>	base pair type of enclosing pair (must be reverse type)
<i>S</i>	integer encoded sequence
<i>ggg</i>	triangular matrix containing g-quadruplex contributions
<i>p</i>	here the 5' position of the gquad is stored
<i>q</i>	here the 3' position of the gquad is stored
<i>P</i>	the datastructure containing the precalculated contibutions

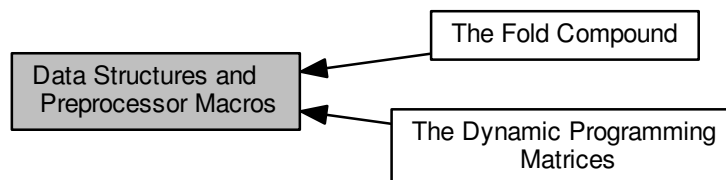
Returns

1 on success, 0 if no gquad found

15.42 Data Structures and Preprocessor Macros

All datastructures and typedefs shared among the Vienna RNA Package can be found here.

Collaboration diagram for Data Structures and Preprocessor Macros:



Modules

- [The Fold Compound](#)
This module provides interfaces that deal with the most basic data structure used in structure predicting and energy evaluating function of the RNAlib.
- [The Dynamic Programming Matrices](#)
This module provides interfaces that deal with creation and destruction of dynamic programming matrices used within the RNAlib.

Files

- file [data_structures.h](#)
Various data structures and pre-processor macros.
- file [dp_matrices.h](#)
Functions to deal with standard dynamic programming (DP) matrices.

Data Structures

- struct [vrna_basepair_s](#)
Base pair data structure used in subopt.c. [More...](#)
- struct [vrna_plist_s](#)
this datastructure is used as input parameter in functions of [PS_dot.h](#) and others [More...](#)
- struct [vrna_cpair_s](#)
this datastructure is used as input parameter in functions of [PS_dot.c](#) [More...](#)
- struct [vrna_color_s](#)
- struct [vrna_data_linear_s](#)
- struct [vrna_sect_s](#)
Stack of partial structures for backtracking. [More...](#)
- struct [vrna_bp_stack_s](#)
Base pair stack element. [More...](#)
- struct [pu_contrib](#)

- contributions to p_u [More...](#)*
- struct [interact](#)
 - interaction data structure for RNAup [More...](#)*
- struct [pu_out](#)
 - Collection of all free_energy of beeing unpaired values for output. [More...](#)*
- struct [constrain](#)
 - constraints for cofolding [More...](#)*
- struct [duplexT](#)
 - Data structure for RNAduplex. [More...](#)*
- struct [node](#)
 - Data structure for RNAsnoop (fold energy list) [More...](#)*
- struct [snoopT](#)
 - Data structure for RNAsnoop. [More...](#)*
- struct [dupVar](#)
 - Data structure used in RNAPkplex. [More...](#)*

Typedefs

- typedef struct [vrna_basepair_s](#) [vrna_basepair_t](#)
 - Typename for the base pair representing data structure [vrna_basepair_s](#).*
- typedef struct [vrna_plist_s](#) [vrna_plist_t](#)
 - Typename for the base pair list representing data structure [vrna_plist_s](#).*
- typedef struct [vrna_bp_stack_s](#) [vrna_bp_stack_t](#)
 - Typename for the base pair stack representing data structure [vrna_bp_stack_s](#).*
- typedef struct [vrna_cpair_s](#) [vrna_cpair_t](#)
 - Typename for data structure [vrna_cpair_s](#).*
- typedef struct [vrna_sect_s](#) [vrna_sect_t](#)
 - Typename for stack of partial structures [vrna_sect_s](#).*
- typedef double [FLT_OR_DBL](#)
 - Typename for floating point number in partition function computations.*
- typedef struct [vrna_basepair_s](#) [PAIR](#)
 - Old typename of [vrna_basepair_s](#).*
- typedef struct [vrna_plist_s](#) [plist](#)
 - Old typename of [vrna_plist_s](#).*
- typedef struct [vrna_cpair_s](#) [cpair](#)
 - Old typename of [vrna_cpair_s](#).*
- typedef struct [vrna_sect_s](#) [sect](#)
 - Old typename of [vrna_sect_s](#).*
- typedef struct [vrna_bp_stack_s](#) [bondT](#)
 - Old typename of [vrna_bp_stack_s](#).*
- typedef struct [pu_contrib](#) [pu_contrib](#)
 - contributions to p_u*
- typedef struct [interact](#) [interact](#)
 - interaction data structure for RNAup*
- typedef struct [pu_out](#) [pu_out](#)
 - Collection of all free_energy of beeing unpaired values for output.*
- typedef struct [constrain](#) [constrain](#)
 - constraints for cofolding*
- typedef struct [node](#) [folden](#)
 - Data structure for RNAsnoop (fold energy list)*
- typedef struct [dupVar](#) [dupVar](#)
 - Data structure used in RNAPkplex.*

Functions

- void [vrna_C11_features](#) (void)

Dummy symbol to check whether the library was build using C11/C++11 features.

15.42.1 Detailed Description

All datastructures and typedefs shared among the Vienna RNA Package can be found [here](#).

15.42.2 Data Structure Documentation

15.42.2.1 struct vrna_basepair_s

Base pair data structure used in subopt.c.

15.42.2.2 struct vrna_plist_s

this datastructure is used as input parameter in functions of [PS_dot.h](#) and others

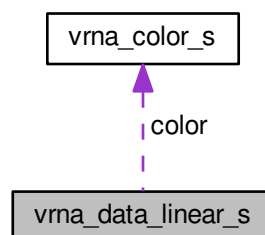
15.42.2.3 struct vrna_cpair_s

this datastructure is used as input parameter in functions of PS_dot.c

15.42.2.4 struct vrna_color_s

15.42.2.5 struct vrna_data_linear_s

Collaboration diagram for vrna_data_linear_s:



15.42.2.6 struct vrna_sect_s

Stack of partial structures for backtracking.

15.42.2.7 struct vrna_bp_stack_s

Base pair stack element.

15.42.2.8 struct pu_contrib

contributions to p_u

Data Fields

- double ** [H](#)
hairpin loops
- double ** [I](#)
interior loops
- double ** [M](#)
multi loops
- double ** [E](#)
exterior loop
- int [length](#)
length of the input sequence
- int [w](#)
longest unpaired region

15.42.2.9 struct interact

interaction data structure for RNAup

Data Fields

- double * [Pi](#)
probabilities of interaction
- double * [Gi](#)
free energies of interaction
- double [Gikjl](#)
full free energy for interaction between $[k,i]$ $k < i$ in longer seq and $[j,l]$ $j < l$ in shorter seq
- double [Gikjl_wo](#)
Gikjl without contributions for prob_unpaired.
- int [i](#)
 $k < i$ in longer seq
- int [k](#)
 $k < i$ in longer seq
- int [j](#)
 $j < l$ in shorter seq
- int [l](#)
 $j < l$ in shorter seq
- int [length](#)
length of longer sequence

15.42.2.10 struct pu_out

Collection of all free_energy of beeing unpaired values for output.

Data Fields

- int `len`
sequence length
- int `u_vals`
number of different -u values
- int `contribs`
[-c "SHIME"]
- char ** `header`
header line
- double ** `u_values`
*(the -u values * [-c "SHIME"]) * seq len*

15.42.2.11 struct constrain

constraints for cofolding

15.42.2.12 struct duplexT

Data structure for RNAduplex.

15.42.2.13 struct node

Data structure for RNAsnoop (fold energy list)

Collaboration diagram for node:



15.42.2.14 struct snoopT

Data structure for RNAsnoop.

15.42.2.15 struct dupVar

Data structure used in RNAppkplex.

15.42.3 Typedef Documentation

15.42.3.1 typedef struct vrna_basepair_s PAIR

```
#include <ViennaRNA/data_structures.h>
```

Old typename of [vrna_basepair_s](#).

Deprecated Use [vrna_basepair_t](#) instead!

15.42.3.2 typedef struct vrna_plist_s plist

```
#include <ViennaRNA/data_structures.h>
```

Old typename of [vrna_plist_s](#).

Deprecated Use [vrna_plist_t](#) instead!

15.42.3.3 typedef struct vrna_cpair_s cpair

```
#include <ViennaRNA/data_structures.h>
```

Old typename of [vrna_cpair_s](#).

Deprecated Use [vrna_cpair_t](#) instead!

15.42.3.4 typedef struct vrna_sect_s sect

```
#include <ViennaRNA/data_structures.h>
```

Old typename of [vrna_sect_s](#).

Deprecated Use [vrna_sect_t](#) instead!

15.42.3.5 typedef struct vrna_bp_stack_s bondT

```
#include <ViennaRNA/data_structures.h>
```

Old typename of `vrna_bp_stack_s`.

Deprecated Use `vrna_bp_stack_t` instead!

15.42.4 Function Documentation

15.42.4.1 void vrna_C11_features (void)

```
#include <ViennaRNA/data_structures.h>
```

Dummy symbol to check whether the library was build using C11/C++11 features.

By default, several data structures of our new v3.0 API use C11/C++11 features, such as unnamed unions, unnamed structs. However, these features can be deactivated at compile time to allow building the library and executables with compilers that do not support these features.

Now, the problem arises that once our static library is compiled and a third-party application is supposed to link against it, it needs to know, at compile time, how to correctly address particular data structures. This is usually implicitly taken care of through the API exposed in our header files. Unfortunately, we had some preprocessor directives in our header files that changed the API depending on the capabilities of the compiler the third-party application is build with. This in turn prohibited the use of an RNAlib compiled without C11/C++11 support in a program that compiles/links with enabled C11/C++11 support and vice-versa.

Therefore, we introduce this dummy symbol which can be used to check, whether the static library was build with C11/C++11 features.

Note

If the symbol is present, the library was build with enabled C11/C++11 features support and no action is required. However, if the symbol is missing in RNAlib $\geq 2.2.9$, programs that link to RNAlib must define a pre-processor identifier `VRNA_DISABLE_C11_FEATURES` before including any ViennaRNA Package header file, for instance by adding a `CPPFLAG`

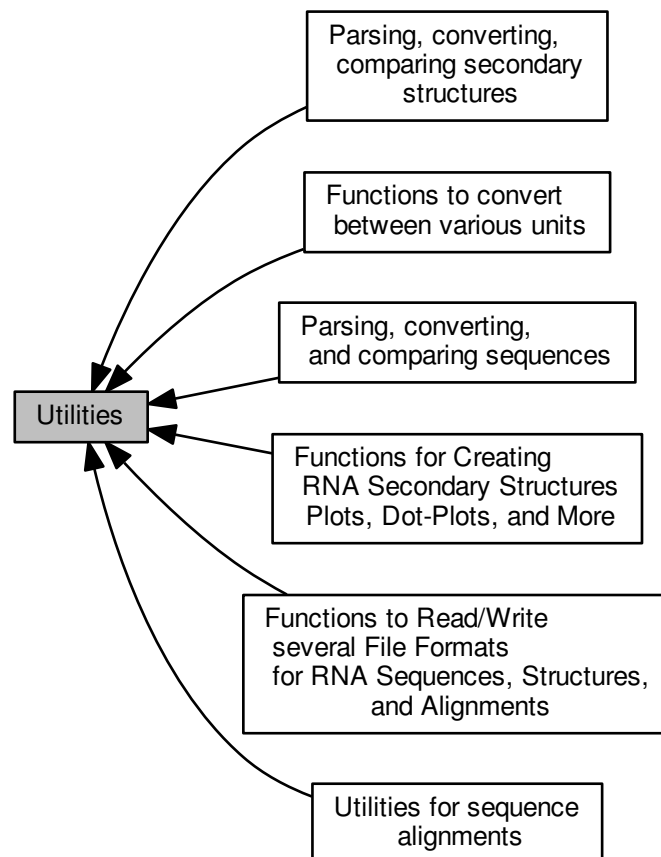
```
00001 CPPFLAGS+=-DVRNA_DISABLE_C11_FEATURES
```

Since

v2.2.9

15.43 Utilities

Collaboration diagram for Utilities:



Modules

- [Parsing, converting, and comparing sequences](#)
- [Parsing, converting, comparing secondary structures](#)
- [Utilities for sequence alignments](#)
- [Functions to Read/Write several File Formats for RNA Sequences, Structures, and Alignments](#)

Functions dealing with file formats for RNA sequences, structures, and alignments.

- [Functions for Creating RNA Secondary Structures Plots, Dot-Plots, and More](#)
- [Functions to convert between various units](#)

Files

- file [aln_util.h](#)

Various utility- and helper-functions for sequence alignments and comparative structure prediction.

- file [alphabet.h](#)
Functions to process, convert, and generally handle different nucleotide and/or base pair alphabets.
- file [combinatorics.h](#)
Various implementations that deal with combinatorial aspects of RNA/DNA folding.
- file [string_utils.h](#)
General utility- and helper-functions for RNA sequence and structure strings used throughout the ViennaRNA Package.
- file [structure_utils.h](#)
Various utility- and helper-functions for secondary structure parsing, converting, etc.
- file [utils.h](#)
General utility- and helper-functions used throughout the ViennaRNA Package.

- `char * vrna_ptypes` (const short *S, `vrna_md_t` *md)
Get an array of the numerical encoding for each possible base pair (i,j)
- `short * vrna_seq_encode` (const char *sequence, `vrna_md_t` *md)
Get a numerical representation of the nucleotide sequence.
- `short * vrna_seq_encode_simple` (const char *sequence, `vrna_md_t` *md)
Get a numerical representation of the nucleotide sequence (simple version)
- `int vrna_nucleotide_encode` (char c, `vrna_md_t` *md)
Encode a nucleotide character to numerical value.
- `char vrna_nucleotide_decode` (int enc, `vrna_md_t` *md)
Decode a numerical representation of a nucleotide back into nucleotide alphabet.

- `unsigned int ** vrna_enumerate_necklaces` (const unsigned int *type_counts)
Enumerate all necklaces with fixed content.

- `void * vrna_alloc` (unsigned size)
Allocate space safely.
- `void * vrna_realloc` (void *p, unsigned size)
Reallocate space safely.
- `void vrna_message_error` (const char *format,...)
Print an error message and die.
- `void vrna_message_verror` (const char *format, va_list args)
Print an error message and die.
- `void vrna_message_warning` (const char *format,...)
Print a warning message.
- `void vrna_message_vwarning` (const char *format, va_list args)
Print a warning message.
- `void vrna_message_info` (FILE *fp, const char *format,...)
Print an info message.
- `void vrna_message_vinfo` (FILE *fp, const char *format, va_list args)
Print an info message.
- `void vrna_init_rand` (void)
Initialize seed for random number generator.
- `double vrna_urn` (void)
get a random number from [0..1]
- `int vrna_int_urn` (int from, int to)
Generates a pseudo random integer in a specified range.
- `char * vrna_time_stamp` (void)

Get a timestamp.

- unsigned int `get_input_line` (char **string, unsigned int options)
- void `vrna_message_input_seq_simple` (void)

Print a line to stdout that asks for an input sequence.

- void `vrna_message_input_seq` (const char *s)

Print a line with a user defined string and a ruler to stdout.

- int * `vrna_idx_row_wise` (unsigned int length)

Get an index mapper array (iindx) for accessing the energy matrices, e.g. in partition function related functions.

- int * `vrna_idx_col_wise` (unsigned int length)

Get an index mapper array (indx) for accessing the energy matrices, e.g. in MFE related functions.

- #define `VRNA_INPUT_ERROR` 1U

Output flag of `get_input_line()`: "An ERROR has occurred, maybe EOF".

- #define `VRNA_INPUT_QUIT` 2U

Output flag of `get_input_line()`: "the user requested quitting the program".

- #define `VRNA_INPUT_MISC` 4U

Output flag of `get_input_line()`: "something was read".

- #define `VRNA_INPUT_FASTA_HEADER` 8U

Input/Output flag of `get_input_line()`:

if used as input option this tells `get_input_line()` that the data to be read should comply with the FASTA format.

- #define `VRNA_INPUT_CONSTRAINT` 32U

Input flag for `get_input_line()`:

Tell `get_input_line()` that we assume to read a structure constraint.

- #define `VRNA_INPUT_NO_TRUNCATION` 256U

Input switch for `get_input_line()`: "do not truncate the line by eliminating white spaces at end of line".

- #define `VRNA_INPUT_NO_REST` 512U

Input switch for `vrna_file_fasta_read_record()`: "do fill rest array".

- #define `VRNA_INPUT_NO_SPAN` 1024U

Input switch for `vrna_file_fasta_read_record()`: "never allow data to span more than one line".

- #define `VRNA_INPUT_NOSKIP_BLANK_LINES` 2048U

Input switch for `vrna_file_fasta_read_record()`: "do not skip empty lines".

- #define `VRNA_INPUT_BLANK_LINE` 4096U

Output flag for `vrna_file_fasta_read_record()`: "read an empty line".

- #define `VRNA_INPUT_NOSKIP_COMMENTS` 128U

Input switch for `get_input_line()`: "do not skip comment lines".

- #define `VRNA_INPUT_COMMENT` 8192U

Output flag for `vrna_file_fasta_read_record()`: "read a comment".

- #define `MIN2(A, B)` ((A) < (B) ? (A) : (B))

Get the minimum of two comparable values.

- #define `MAX2(A, B)` ((A) > (B) ? (A) : (B))

Get the maximum of two comparable values.

- #define `MIN3(A, B, C)` (MIN2((MIN2((A),(B))), (C)))

Get the minimum of three comparable values.

- #define `MAX3(A, B, C)` (MAX2((MAX2((A),(B))), (C)))

Get the maximum of three comparable values.

- unsigned short `xsubi` [3]

Current 48 bit random number.

15.43.1 Detailed Description

15.43.2 Macro Definition Documentation

15.43.2.1 `#define VRNA_INPUT_FASTA_HEADER 8U`

```
#include <ViennaRNA/utils.h>
```

Input/Output flag of `get_input_line()`:

if used as input option this tells `get_input_line()` that the data to be read should comply with the FASTA format.

the function will return this flag if a fasta header was read

15.43.2.2 `#define VRNA_INPUT_CONSTRAINT 32U`

```
#include <ViennaRNA/utils.h>
```

Input flag for `get_input_line()`:

Tell `get_input_line()` that we assume to read a structure constraint.

15.43.3 Function Documentation

15.43.3.1 `unsigned int ** vrna_enumerate_necklaces (const unsigned int * type_counts)`

```
#include <ViennaRNA/combinatorics.h>
```

Enumerate all necklaces with fixed content.

This function implements *A fast algorithm to generate necklaces with fixed content* as published by Joe Sawada in 2003 [16].

The function receives a list of counts (the elements on the necklace) for each type of object within a necklace. The list starts at index 0 and ends with an entry that has a count of 0. The algorithm then enumerates all non-cyclic permutations of the content, returned as a list of necklaces. This list, again, is zero-terminated, i.e. the last entry of the list is a `NULL` pointer.

Parameters

<code>type_counts</code>	A 0-terminated list of entity counts
--------------------------	--------------------------------------

Returns

A list of all non-cyclic permutations of the entities

SWIG Wrapper Notes This function is available as global function `enumerate_necklaces()` which accepts lists input, and produces list of lists output.

15.43.3.2 `char* vrna_ptypes (const short * S, vrna_md_t * md)`

```
#include <ViennaRNA/alphabet.h>
```

Get an array of the numerical encoding for each possible base pair (i,j)

Note

This array is always indexed in column-wise order, in contrast to previously different indexing between mfe and pf variants!

See also

[vrna_idx_col_wise\(\)](#), [vrna_fold_compound_t](#)

15.43.3.3 `int vrna_nucleotide_encode (char c, vrna_md_t * md)`

```
#include <ViennaRNA/alphabet.h>
```

Encode a nucleotide character to numerical value.

This function encodes a nucleotide character to its numerical representation as required by many functions in R_{NALib}.

See also

[vrna_nucleotide_decode\(\)](#), [vrna_seq_encode\(\)](#)

Parameters

<i>c</i>	The nucleotide character to encode
<i>md</i>	The model details that determine the kind of encoding

Returns

The encoded nucleotide

15.43.3.4 `char vrna_nucleotide_decode (int enc, vrna_md_t * md)`

```
#include <ViennaRNA/alphabet.h>
```

Decode a numerical representation of a nucleotide back into nucleotide alphabet.

This function decodes a numerical representation of a nucleotide character back into nucleotide alphabet

See also

[vrna_nucleotide_encode\(\)](#), [vrna_seq_encode\(\)](#)

Parameters

<i>enc</i>	The encoded nucleotide
<i>md</i>	The model details that determine the kind of decoding

Returns

The decoded nucleotide character

15.43.3.5 void* vrna_alloc (unsigned size)

```
#include <ViennaRNA/utils.h>
```

Allocate space safely.

Parameters

<i>size</i>	The size of the memory to be allocated in bytes
-------------	-------------------------------------------------

Returns

A pointer to the allocated memory

15.43.3.6 void* vrna_realloc (void * p, unsigned size)

```
#include <ViennaRNA/utils.h>
```

Reallocate space safely.

Parameters

<i>p</i>	A pointer to the memory region to be reallocated
<i>size</i>	The size of the memory to be allocated in bytes

Returns

A pointer to the newly allocated memory

15.43.3.7 void vrna_message_error (const char * format, ...)

```
#include <ViennaRNA/utils.h>
```

Print an error message and die.

This function is a wrapper to `fprintf(stderr, ...)` that puts a capital **ERROR:** in front of the message and then exits the calling program.

See also

[vrna_message_verror\(\)](#), [vrna_message_warning\(\)](#), [vrna_message_info\(\)](#)

Parameters

<i>format</i>	The error message to be printed
...	Optional arguments for the formatted message string

15.43.3.8 void vrna_message_verror (const char * *format*, va_list *args*)

```
#include <ViennaRNA/utils.h>
```

Print an error message and die.

This function is a wrapper to `vfprintf(stderr, ...)` that puts a capital **ERROR:** in front of the message and then exits the calling program.

See also

[vrna_message_error\(\)](#), [vrna_message_warning\(\)](#), [vrna_message_info\(\)](#)

Parameters

<i>format</i>	The error message to be printed
<i>args</i>	The argument list for the formatted message string

15.43.3.9 void vrna_message_warning (const char * *format*, ...)

```
#include <ViennaRNA/utils.h>
```

Print a warning message.

This function is a wrapper to `fprintf(stderr, ...)` that puts a capital **WARNING:** in front of the message.

See also

[vrna_message_vwarning\(\)](#), [vrna_message_error\(\)](#), [vrna_message_info\(\)](#)

Parameters

<i>format</i>	The warning message to be printed
...	Optional arguments for the formatted message string

15.43.3.10 void vrna_message_vwarning (const char * *format*, va_list *args*)

```
#include <ViennaRNA/utils.h>
```

Print a warning message.

This function is a wrapper to `fprintf(stderr, ...)` that puts a capital **WARNING:** in front of the message.

See also

[vrna_message_vwarning\(\)](#), [vrna_message_error\(\)](#), [vrna_message_info\(\)](#)

Parameters

<i>format</i>	The warning message to be printed
<i>args</i>	The argument list for the formatted message string

15.43.3.11 void `vrna_message_info` (FILE * *fp*, const char * *format*, ...)

```
#include <ViennaRNA/utils.h>
```

Print an info message.

This function is a wrapper to `fprintf(...)`.

See also

[vrna_message_vinfo\(\)](#), [vrna_message_error\(\)](#), [vrna_message_warning\(\)](#)

Parameters

<i>fp</i>	The file pointer where the message is printed to
<i>format</i>	The warning message to be printed
...	Optional arguments for the formatted message string

15.43.3.12 void `vrna_message_vinfo` (FILE * *fp*, const char * *format*, va_list *args*)

```
#include <ViennaRNA/utils.h>
```

Print an info message.

This function is a wrapper to `fprintf(...)`.

See also

[vrna_message_vinfo\(\)](#), [vrna_message_error\(\)](#), [vrna_message_warning\(\)](#)

Parameters

<i>fp</i>	The file pointer where the message is printed to
<i>format</i>	The info message to be printed
<i>args</i>	The argument list for the formatted message string

15.43.3.13 `double vrna_urn (void)`

```
#include <ViennaRNA/utils.h>
```

get a random number from [0..1]

See also

[vrna_int_urn\(\)](#), [vrna_init_rand\(\)](#)

Note

Usually implemented by calling *erand48()*.

Returns

A random number in range [0..1]

15.43.3.14 `int vrna_int_urn (int from, int to)`

```
#include <ViennaRNA/utils.h>
```

Generates a pseudo random integer in a specified range.

See also

[vrna_urn\(\)](#), [vrna_init_rand\(\)](#)

Parameters

<i>from</i>	The first number in range
<i>to</i>	The last number in range

Returns

A pseudo random number in range [from, to]

15.43.3.15 `char* vrna_time_stamp (void)`

```
#include <ViennaRNA/utils.h>
```

Get a timestamp.

Returns a string containing the current date in the format

```
Fri Mar 19 21:10:57 1993
```

Returns

A string containing the timestamp

15.43.3.16 unsigned int get_input_line (char ** *string*, unsigned int *options*)

```
#include <ViennaRNA/utils.h>
```

Retrieve a line from 'stdin' safely while skipping comment characters and other features This function returns the type of input it has read if recognized. An option argument allows one to switch between different reading modes.

Currently available options are:

#VRNA_INPUT_NOPRINT_COMMENTS, [VRNA_INPUT_NOSKIP_COMMENTS](#), #VRNA_INPUT_NOELIM_WS_SUFFIX

pass a collection of options as one value like this:

```
get_input_line(string, option_1 | option_2 | option_n)
```

If the function recognizes the type of input, it will report it in the return value. It also reports if a user defined 'quit' command (-sign on 'stdin') was given. Possible return values are:

[VRNA_INPUT_FASTA_HEADER](#), [VRNA_INPUT_ERROR](#), [VRNA_INPUT_MISC](#), [VRNA_INPUT_QUIT](#)

Parameters

<i>string</i>	A pointer to the character array that contains the line read
<i>options</i>	A collection of options for switching the functions behavior

Returns

A flag with information about what has been read

15.43.3.17 void vrna_message_input_seq_simple (void)

```
#include <ViennaRNA/utils.h>
```

Print a line to *stdout* that asks for an input sequence.

There will also be a ruler (scale line) printed that helps orientation of the sequence positions

15.43.3.18 void vrna_message_input_seq (const char * *s*)

```
#include <ViennaRNA/utils.h>
```

Print a line with a user defined string and a ruler to stdout.

(usually this is used to ask for user input) There will also be a ruler (scale line) printed that helps orientation of the sequence positions

Parameters

<i>s</i>	A user defined string that will be printed to stdout
----------	------------------------------------------------------

15.43.3.19 `int* vrna_idx_row_wise (unsigned int length)`

```
#include <ViennaRNA/utils.h>
```

Get an index mapper array (iindx) for accessing the energy matrices, e.g. in partition function related functions.

Access of a position "(i,j)" is then accomplished by using

```
(i,j) ~ iindx[i]-j
```

This function is necessary as most of the two-dimensional energy matrices are actually one-dimensional arrays throughout the ViennaRNA Package

Consult the implemented code to find out about the mapping formula ;)

See also

[vrna_idx_col_wise\(\)](#)

Parameters

<i>length</i>	The length of the RNA sequence
---------------	--------------------------------

Returns

The mapper array

15.43.3.20 `int* vrna_idx_col_wise (unsigned int length)`

```
#include <ViennaRNA/utils.h>
```

Get an index mapper array (indx) for accessing the energy matrices, e.g. in MFE related functions.

Access of a position "(i,j)" is then accomplished by using

```
(i,j) ~ indx[j]+i
```

This function is necessary as most of the two-dimensional energy matrices are actually one-dimensional arrays throughout the ViennaRNAPackage

Consult the implemented code to find out about the mapping formula ;)

See also

[vrna_idx_row_wise\(\)](#)

Parameters

<i>length</i>	The length of the RNA sequence
---------------	--------------------------------

Returns

The mapper array

15.43.4 Variable Documentation**15.43.4.1 unsigned short xsubi[3]**

```
#include <ViennaRNA/utils.h>
```

Current 48 bit random number.

This variable is used by [vrna_urn\(\)](#). These should be set to some random number seeds before the first call to [vrna_urn\(\)](#).

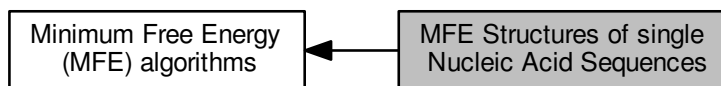
See also

[vrna_urn\(\)](#)

15.44 MFE Structures of single Nucleic Acid Sequences

This module contains all functions and variables related to the calculation of global minimum free energy structures for single sequences.

Collaboration diagram for MFE Structures of single Nucleic Acid Sequences:



Functions

- float [vrna_fold](#) (const char *sequence, char *structure)
Compute Minimum Free Energy (MFE), and a corresponding secondary structure for an RNA sequence.
- float [vrna_circfold](#) (const char *sequence, char *structure)
Compute Minimum Free Energy (MFE), and a corresponding secondary structure for a circular RNA sequence.
- float [fold_par](#) (const char *sequence, char *structure, [vrna_param_t](#) *parameters, int is_constrained, int is_circular)
Compute minimum free energy and an appropriate secondary structure of an RNA sequence.
- float [fold](#) (const char *sequence, char *structure)
Compute minimum free energy and an appropriate secondary structure of an RNA sequence.
- float [circfold](#) (const char *sequence, char *structure)
Compute minimum free energy and an appropriate secondary structure of a circular RNA sequence.
- void [free_arrays](#) (void)
Free arrays for mfe folding.
- void [update_fold_params](#) (void)
Recalculate energy parameters.
- void [update_fold_params_par](#) ([vrna_param_t](#) *parameters)
Recalculate energy parameters.
- void [export_fold_arrays](#) (int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **indx_p, char **ptype_p)
- void [export_fold_arrays_par](#) (int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **indx_p, char **ptype_p, [vrna_param_t](#) **P_p)
- void [export_circfold_arrays](#) (int *Fc_p, int *FcH_p, int *Fcl_p, int *FcM_p, int **fM2_p, int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **indx_p, char **ptype_p)
- void [export_circfold_arrays_par](#) (int *Fc_p, int *FcH_p, int *Fcl_p, int *FcM_p, int **fM2_p, int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **indx_p, char **ptype_p, [vrna_param_t](#) **P_p)
- int [LoopEnergy](#) (int n1, int n2, int type, int type_2, int si1, int sj1, int sp1, int sq1)
- int [HairpinE](#) (int size, int type, int si1, int sj1, const char *string)
- void [initialize_fold](#) (int length)

15.44.1 Detailed Description

This module contains all functions and variables related to the calculation of global minimum free energy structures for single sequences.

The library provides a fast dynamic programming minimum free energy folding algorithm as described by "Zuker & Stiegler (1981)" [24].

15.44.2 Function Documentation

15.44.2.1 `float vrna_fold (const char * sequence, char * structure)`

```
#include <ViennaRNA/fold.h>
```

Compute Minimum Free Energy (MFE), and a corresponding secondary structure for an RNA sequence.

This simplified interface to [vrna_mfe\(\)](#) computes the MFE and, if required, a secondary structure for an RNA sequence using default options. Memory required for dynamic programming (DP) matrices will be allocated and free'd on-the-fly. Hence, after return of this function, the recursively filled matrices are not available any more for any post-processing, e.g. suboptimal backtracking, etc.

Note

In case you want to use the filled DP matrices for any subsequent post-processing step, or you require other conditions than specified by the default model details, use [vrna_mfe\(\)](#), and the data structure [vrna_fold_compound_t](#) instead.

See also

[vrna_circfold\(\)](#), [vrna_mfe\(\)](#), [vrna_fold_compound\(\)](#), [vrna_fold_compound_t](#)

Parameters

<i>sequence</i>	RNA sequence
<i>structure</i>	A pointer to the character array where the secondary structure in dot-bracket notation will be written to

Returns

the minimum free energy (MFE) in kcal/mol

15.44.2.2 `float vrna_circfold (const char * sequence, char * structure)`

```
#include <ViennaRNA/fold.h>
```

Compute Minimum Free Energy (MFE), and a corresponding secondary structure for a circular RNA sequence.

This simplified interface to [vrna_mfe\(\)](#) computes the MFE and, if required, a secondary structure for a circular RNA sequence using default options. Memory required for dynamic programming (DP) matrices will be allocated and free'd on-the-fly. Hence, after return of this function, the recursively filled matrices are not available any more for any post-processing, e.g. suboptimal backtracking, etc.

Folding of circular RNA sequences is handled as a post-processing step of the forward recursions. See [9] for further details.

Note

In case you want to use the filled DP matrices for any subsequent post-processing step, or you require other conditions than specified by the default model details, use [vrna_mfe\(\)](#), and the data structure [vrna_fold_compound_t](#) instead.

See also

[vrna_fold\(\)](#), [vrna_mfe\(\)](#), [vrna_fold_compound\(\)](#), [vrna_fold_compound_t](#)

Parameters

<i>sequence</i>	RNA sequence
<i>structure</i>	A pointer to the character array where the secondary structure in dot-bracket notation will be written to

Returns

the minimum free energy (MFE) in kcal/mol

15.44.2.3 `float fold_par (const char * sequence, char * structure, vrna_param_t * parameters, int is_constrained, int is_circular)`

```
#include <ViennaRNA/fold.h>
```

Compute minimum free energy and an appropriate secondary structure of an RNA sequence.

The first parameter given, the RNA sequence, must be *uppercase* and should only contain an alphabet Σ that is understood by the RNAlib

(e.g. $\Sigma = \{A, U, C, G\}$)

The second parameter, *structure*, must always point to an allocated block of memory with a size of at least `strlen(sequence) + 1`

If the third parameter is NULL, global model detail settings are assumed for the folding recursions. Otherwise, the provided parameters are used.

The fourth parameter indicates whether a secondary structure constraint in enhanced dot-bracket notation is passed through the structure parameter or not. If so, the characters "`| x < >`" are recognized to mark bases that are paired, unpaired, paired upstream, or downstream, respectively. Matching brackets "`()`" denote base pairs, dots "`.`" are used for unconstrained bases.

To indicate that the RNA sequence is circular and thus has to be post-processed, set the last parameter to non-zero

After a successful call of `fold_par()`, a backtracked secondary structure (in dot-bracket notation) that exhibits the minimum of free energy will be written to the memory *structure* is pointing to. The function returns the minimum of free energy for any fold of the sequence given.

Note

OpenMP: Passing NULL to the 'parameters' argument involves access to several global model detail variables and thus is not to be considered threadsafe

Deprecated use `vrna_mfe()` instead!

See also

`vrna_mfe()`, `fold()`, `circfold()`, `vrna_md_t`, `set_energy_model()`, `get_scaled_parameters()`

Parameters

<i>sequence</i>	RNA sequence
<i>structure</i>	A pointer to the character array where the secondary structure in dot-bracket notation will be written to
<i>parameters</i>	A data structure containing the pre-scaled energy contributions and the model details. (NULL may be passed, see OpenMP notes above)
<i>is_constrained</i>	Switch to indicate that a structure constraint is passed via the structure argument (0==off)
<i>is_circular</i>	Switch to (de-)activate post-processing steps in case RNA sequence is circular (0==off)

Returns

the minimum free energy (MFE) in kcal/mol

15.44.2.4 float fold (const char * *sequence*, char * *structure*)

```
#include <ViennaRNA/fold.h>
```

Compute minimum free energy and an appropriate secondary structure of an RNA sequence.

This function essentially does the same thing as [fold_par\(\)](#). However, it takes its model details, i.e. [temperature](#), [dangles](#), [tetra_loop](#), [noGU](#), [no_closingGU](#), [fold_constrained](#), [noLonelyPairs](#) from the current global settings within the library

Deprecated use [vrna_fold\(\)](#), or [vrna_mfe\(\)](#) instead!

See also

[fold_par\(\)](#), [circfold\(\)](#)

Parameters

<i>sequence</i>	RNA sequence
<i>structure</i>	A pointer to the character array where the secondary structure in dot-bracket notation will be written to

Returns

the minimum free energy (MFE) in kcal/mol

15.44.2.5 float circfold (const char * *sequence*, char * *structure*)

```
#include <ViennaRNA/fold.h>
```

Compute minimum free energy and an appropriate secondary structure of a circular RNA sequence.

This function essentially does the same thing as [fold_par\(\)](#). However, it takes its model details, i.e. [temperature](#), [dangles](#), [tetra_loop](#), [noGU](#), [no_closingGU](#), [fold_constrained](#), [noLonelyPairs](#) from the current global settings within the library

Deprecated Use [vrna_circfold\(\)](#), or [vrna_mfe\(\)](#) instead!

See also

[fold_par\(\)](#), [circfold\(\)](#)

Parameters

<i>sequence</i>	RNA sequence
<i>structure</i>	A pointer to the character array where the secondary structure in dot-bracket notation will be written to

Returns

the minimum free energy (MFE) in kcal/mol

15.44.2.6 void free_arrays (void)

```
#include <ViennaRNA/fold.h>
```

Free arrays for mfe folding.

Deprecated See [vrna_fold\(\)](#), [vrna_circfold\(\)](#), or [vrna_mfe\(\)](#) and [vrna_fold_compound_t](#) for the usage of the new API!

15.44.2.7 void update_fold_params (void)

```
#include <ViennaRNA/fold.h>
```

Recalculate energy parameters.

Deprecated For non-default model settings use the new API with [vrna_params_subst\(\)](#) and [vrna_mfe\(\)](#) instead!

15.44.2.8 void update_fold_params_par (vrna_param_t * parameters)

```
#include <ViennaRNA/fold.h>
```

Recalculate energy parameters.

Deprecated For non-default model settings use the new API with [vrna_params_subst\(\)](#) and [vrna_mfe\(\)](#) instead!

15.44.2.9 void export_fold_arrays (int ** f5_p, int ** c_p, int ** fML_p, int ** fM1_p, int ** indx_p, char ** ptype_p)

```
#include <ViennaRNA/fold.h>
```

Deprecated See [vrna_mfe\(\)](#) and [vrna_fold_compound_t](#) for the usage of the new API!

15.44.2.10 void export_fold_arrays_par (int ** *f5_p*, int ** *c_p*, int ** *fML_p*, int ** *fM1_p*, int ** *indx_p*, char ** *ptype_p*,
vrna_param_t ** *P_p*)

#include <ViennaRNA/fold.h>

Deprecated See [vrna_mfe\(\)](#) and [vrna_fold_compound_t](#) for the usage of the new API!

15.44.2.11 void export_circfold_arrays (int * *Fc_p*, int * *FcH_p*, int * *Fcl_p*, int * *FcM_p*, int ** *fM2_p*, int ** *f5_p*, int **
c_p, int ** *fML_p*, int ** *fM1_p*, int ** *indx_p*, char ** *ptype_p*)

#include <ViennaRNA/fold.h>

Deprecated See [vrna_mfe\(\)](#) and [vrna_fold_compound_t](#) for the usage of the new API!

15.44.2.12 void export_circfold_arrays_par (int * *Fc_p*, int * *FcH_p*, int * *Fcl_p*, int * *FcM_p*, int ** *fM2_p*, int ** *f5_p*, int
** *c_p*, int ** *fML_p*, int ** *fM1_p*, int ** *indx_p*, char ** *ptype_p*, vrna_param_t ** *P_p*)

#include <ViennaRNA/fold.h>

Deprecated See [vrna_mfe\(\)](#) and [vrna_fold_compound_t](#) for the usage of the new API!

15.44.2.13 int LoopEnergy (int *n1*, int *n2*, int *type*, int *type_2*, int *si1*, int *sj1*, int *sp1*, int *sq1*)

#include <ViennaRNA/fold.h>

Deprecated {This function is deprecated and will be removed soon. Use [E_IntLoop\(\)](#) instead!}

15.44.2.14 int HairpinE (int *size*, int *type*, int *si1*, int *sj1*, const char * *string*)

#include <ViennaRNA/fold.h>

Deprecated {This function is deprecated and will be removed soon. Use [E_Hairpin\(\)](#) instead!}

15.44.2.15 void initialize_fold (int *length*)

#include <ViennaRNA/fold.h>

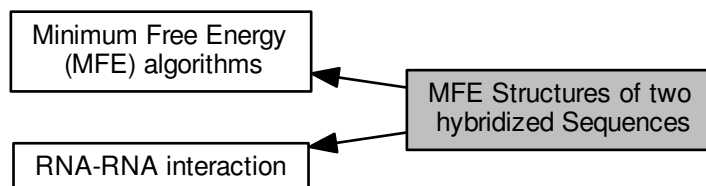
Allocate arrays for folding

Deprecated See [vrna_mfe\(\)](#) and [vrna_fold_compound_t](#) for the usage of the new API!

15.45 MFE Structures of two hybridized Sequences

MFE version of cofolding routines This file includes (almost) all function declarations within the **RNALib** that are related to MFE Cofolding... This also includes the Zuker suboptimals calculations, since they are implemented using the cofold routines.

Collaboration diagram for MFE Structures of two hybridized Sequences:



Functions

- float [vrna_cofold](#) (const char *sequence, char *structure)
Compute Minimum Free Energy (MFE), and a corresponding secondary structure for two dimerized RNA sequences.
- float [cofold](#) (const char *sequence, char *structure)
Compute the minimum free energy of two interacting RNA molecules.
- float [cofold_par](#) (const char *string, char *structure, [vrna_param_t](#) *parameters, int is_constrained)
Compute the minimum free energy of two interacting RNA molecules.
- void [free_co_arrays](#) (void)
Free memory occupied by [cofold\(\)](#)
- void [update_cofold_params](#) (void)
Recalculate parameters.
- void [update_cofold_params_par](#) ([vrna_param_t](#) *parameters)
Recalculate parameters.
- void [export_cofold_arrays_gq](#) (int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **fc_p, int **ggg_p, int **indx_p, char **ptype_p)
Export the arrays of partition function cofold (with gquadruplex support)
- void [export_cofold_arrays](#) (int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **fc_p, int **indx_p, char **ptype_p)
Export the arrays of partition function cofold.
- void [get_monomere_mfes](#) (float *e1, float *e2)
get_monomer_free_energies
- void [initialize_cofold](#) (int length)
- float [vrna_mfe_dimer](#) ([vrna_fold_compound_t](#) *vc, char *structure)
Compute the minimum free energy of two interacting RNA molecules.

15.45.1 Detailed Description

MFE version of cofolding routines This file includes (almost) all function declarations within the **RNALib** that are related to MFE Cofolding... This also includes the Zuker suboptimals calculations, since they are implemented using the cofold routines.

15.45.2 Function Documentation

15.45.2.1 float vrna_cofold (const char * *sequence*, char * *structure*)

```
#include <ViennaRNA/cofold.h>
```

Compute Minimum Free Energy (MFE), and a corresponding secondary structure for two dimerized RNA sequences.

This simplified interface to [vrna_mfe\(\)](#) computes the MFE and, if required, a secondary structure for two RNA sequences upon dimerization using default options. Memory required for dynamic programming (DP) matrices will be allocated and free'd on-the-fly. Hence, after return of this function, the recursively filled matrices are not available any more for any post-processing, e.g. suboptimal backtracking, etc.

Note

In case you want to use the filled DP matrices for any subsequent post-processing step, or you require other conditions than specified by the default model details, use [vrna_mfe\(\)](#), and the data structure [vrna_fold_compound_t](#) instead.

See also

[vrna_mfe_dimer\(\)](#), [vrna_fold_compound\(\)](#), [vrna_fold_compound_t](#), [vrna_cut_point_insert\(\)](#)

Parameters

<i>sequence</i>	two RNA sequences separated by the '&' character
<i>structure</i>	A pointer to the character array where the secondary structure in dot-bracket notation will be written to

Returns

the minimum free energy (MFE) in kcal/mol

15.45.2.2 float cofold (const char * *sequence*, char * *structure*)

```
#include <ViennaRNA/cofold.h>
```

Compute the minimum free energy of two interacting RNA molecules.

The code is analog to the [fold\(\)](#) function. If [cut_point](#) == -1 results should be the same as with [fold\(\)](#).

Deprecated use [vrna_mfe_dimer\(\)](#) instead

Parameters

<i>sequence</i>	The two sequences concatenated
<i>structure</i>	Will hold the barcket dot structure of the dimer molecule

Returns

minimum free energy of the structure

15.45.2.3 `float cofold_par (const char * string, char * structure, vrna_param_t * parameters, int is_constrained)`

```
#include <ViennaRNA/cofold.h>
```

Compute the minimum free energy of two interacting RNA molecules.

Deprecated use `vrna_mfe_dimer()` instead

15.45.2.4 `void free_co_arrays (void)`

```
#include <ViennaRNA/cofold.h>
```

Free memory occupied by `cofold()`

Deprecated This function will only free memory allocated by a prior call of `cofold()` or `cofold_par()`. See [vrna_mfe_dimer\(\)](#) for how to use the new API

Note

folding matrices now reside in the fold compound, and should be free'd there

See also

`vrna_fc_destroy()`, [vrna_mfe_dimer\(\)](#)

15.45.2.5 `void update_cofold_params (void)`

```
#include <ViennaRNA/cofold.h>
```

Recalculate parameters.

Deprecated See [vrna_params_subst\(\)](#) for an alternative using the new API

15.45.2.6 `void update_cofold_params_par (vrna_param_t * parameters)`

```
#include <ViennaRNA/cofold.h>
```

Recalculate parameters.

Deprecated See [vrna_params_subst\(\)](#) for an alternative using the new API

15.45.2.7 `void export_cofold_arrays_gg (int ** f5_p, int ** c_p, int ** fML_p, int ** fM1_p, int ** fc_p, int ** ggg_p, int ** indx_p, char ** ptype_p)`

```
#include <ViennaRNA/cofold.h>
```

Export the arrays of partition function cofold (with gquadruplex support)

Export the cofold arrays for use e.g. in the concentration Computations or suboptimal secondary structure backtracking

Deprecated folding matrices now reside within the fold compound. Thus, this function will only work in conjunction with a prior call to `cofold()` or `cofold_par()`

See also

[vrna_mfe_dimer\(\)](#) for the new API

Parameters

<i>f5_p</i>	A pointer to the 'f5' array, i.e. array containing best free energy in interval [1..j]
<i>c_p</i>	A pointer to the 'c' array, i.e. array containing best free energy in interval [i..j] given that i pairs with j
<i>fML_p</i>	A pointer to the 'M' array, i.e. array containing best free energy in interval [i..j] for any multiloop segment with at least one stem
<i>fM1_p</i>	A pointer to the 'M1' array, i.e. array containing best free energy in interval [i..j] for multiloop segment with exactly one stem
<i>fc_p</i>	A pointer to the 'fc' array, i.e. array ...
<i>ggg_p</i>	A pointer to the 'ggg' array, i.e. array containing best free energy of a gquadruplex delimited by [i..j]
<i>indx_p</i>	A pointer to the indexing array used for accessing the energy matrices
<i>ptype_p</i>	A pointer to the ptype array containing the base pair types for each possibility (i,j)

15.45.2.8 `void export_cofold_arrays (int ** f5_p, int ** c_p, int ** fML_p, int ** fM1_p, int ** fc_p, int ** indx_p, char ** ptype_p)`

```
#include <ViennaRNA/cofold.h>
```

Export the arrays of partition function cofold.

Export the cofold arrays for use e.g. in the concentration Computations or suboptimal secondary structure backtracking

Deprecated folding matrices now reside within the `vrna_fold_compound_t`. Thus, this function will only work in conjunction with a prior call to the deprecated functions `cofold()` or `cofold_par()`

See also

[vrna_mfe_dimer\(\)](#) for the new API

Parameters

<i>f5_p</i>	A pointer to the 'f5' array, i.e. array containing best free energy in interval [1..j]
<i>c_p</i>	A pointer to the 'c' array, i.e. array containing best free energy in interval [i..j] given that i pairs with j
<i>fML_p</i>	A pointer to the 'M' array, i.e. array containing best free energy in interval [i..j] for any multiloop segment with at least one stem
<i>fM1_p</i>	A pointer to the 'M1' array, i.e. array containing best free energy in interval [i..j] for multiloop segment with exactly one stem
<i>fc_p</i>	A pointer to the 'fc' array, i.e. array ...
<i>indx_p</i>	A pointer to the indexing array used for accessing the energy matrices
<i>pptype←_p</i>	A pointer to the ptype array containing the base pair types for each possibility (i,j)

15.45.2.9 void `get_monomere_mfes (float * e1, float * e2)`

```
#include <ViennaRNA/cofold.h>
```

`get_monomer_free_energies`

Export monomer free energies out of cofold arrays

Deprecated {This function is obsolete and will be removed soon!}

Parameters

<i>e1</i>	A pointer to a variable where the energy of molecule A will be written to
<i>e2</i>	A pointer to a variable where the energy of molecule B will be written to

15.45.2.10 void `initialize_cofold (int length)`

```
#include <ViennaRNA/cofold.h>
```

allocate arrays for folding

Deprecated {This function is obsolete and will be removed soon!}

15.45.2.11 float `vrna_mfe_dimer (vrna_fold_compound_t * vc, char * structure)`

```
#include <ViennaRNA/mfe.h>
```

Compute the minimum free energy of two interacting RNA molecules.

The code is analog to the `vrna_mfe()` function.

Parameters

<i>vc</i>	fold compound
<i>structure</i>	Will hold the barcket dot structure of the dimer molecule

Returns

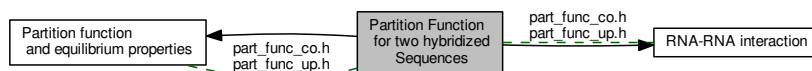
minimum free energy of the structure

SWIG Wrapper Notes This function is attached as method **mfe_dimer()** to objects of type *fold_compound*

15.46 Partition Function for two hybridized Sequences

Partition Function Cofolding.

Collaboration diagram for Partition Function for two hybridized Sequences:



Files

- file [part_func_co.h](#)
Partition function for two RNA sequences.
- file [part_func_up.h](#)
Implementations for accessibility and RNA-RNA interaction as a stepwise process.

Data Structures

- struct [vrna_dimer_pf_s](#)
Data structure returned by [vrna_pf_dimer\(\)](#) [More...](#)
- struct [vrna_dimer_conc_s](#)
Data structure for concentration dependency computations. [More...](#)

Typedefs

- typedef struct [vrna_dimer_pf_s](#) [vrna_dimer_pf_t](#)
Typename for the data structure that stores the dimer partition functions, [vrna_dimer_pf_s](#), as returned by [vrna_pf_dimer\(\)](#)
- typedef struct [vrna_dimer_conc_s](#) [vrna_dimer_conc_t](#)
Typename for the data structure that stores the dimer concentrations, [vrna_dimer_conc_s](#), as required by [vrna_pf_dimer_concentration\(\)](#)
- typedef struct [vrna_dimer_pf_s](#) [cofoldF](#)
Backward compatibility typedef for [vrna_dimer_pf_s](#).
- typedef struct [vrna_dimer_conc_s](#) [ConcEnt](#)
Backward compatibility typedef for [vrna_dimer_conc_s](#).

Functions

- [vrna_dimer_pf_t](#) [vrna_pf_dimer](#) ([vrna_fold_compound_t](#) *vc, char *structure)
Calculate partition function and base pair probabilities of nucleic acid/nucleic acid dimers.
- void [vrna_pf_dimer_probs](#) (double FAB, double FA, double FB, [vrna_plist_t](#) *prAB, const [vrna_plist_t](#) *prA, const [vrna_plist_t](#) *prB, int Alength, const [vrna_exp_param_t](#) *exp_params)
Compute Boltzmann probabilities of dimerization without homodimers.
- [vrna_dimer_conc_t](#) * [vrna_pf_dimer_concentrations](#) (double FcAB, double FcAA, double FcBB, double FEA, double FEB, const double *startconc, const [vrna_exp_param_t](#) *exp_params)
Given two start monomer concentrations a and b, compute the concentrations in thermodynamic equilibrium of all dimers and the monomers.

Variables

- int [mirnatog](#)
Toggles no intrabp in 2nd mol.
- double [F_monomer](#) [2]
Free energies of the two monomers.

15.46.1 Detailed Description

Partition Function Cofolding.

To simplify the implementation the partition function computation is done internally in a null model that does not include the duplex initiation energy, i.e. the entropic penalty for producing a dimer from two monomers). The resulting free energies and pair probabilities are initially relative to that null model. In a second step the free energies can be corrected to include the dimerization penalty, and the pair probabilities can be divided into the conditional pair probabilities given that a re dimer is formed or not formed. See [2] for further details.

As for folding one RNA molecule, this computes the partition function of all possible structures and the base pair probabilities. Uses the same global [pf_scale](#) variable to avoid overflows.

To simplify the implementation the partition function computation is done internally in a null model that does not include the duplex initiation energy, i.e. the entropic penalty for producing a dimer from two monomers). The resulting free energies and pair probabilities are initially relative to that null model. In a second step the free energies can be corrected to include the dimerization penalty, and the pair probabilities can be divided into the conditional pair probabilities given that a re dimer is formed or not formed.

After computing the partition functions of all possible dimers one can compute the probabilities of base pairs, the concentrations out of start concentrations and sofar and soaway.

Dimer formation is inherently concentration dependent. Given the free energies of the monomers A and B and dimers AB, AA, and BB one can compute the equilibrium concentrations, given input concentrations of A and B, see e.g. Dimitrov & Zuker (2004)

15.46.2 Data Structure Documentation

15.46.2.1 struct vrna_dimer_pf_s

Data structure returned by [vrna_pf_dimer\(\)](#)

Data Fields

- double [F0AB](#)
Null model without DuplexInit.
- double [FAB](#)
all states with DuplexInit correction
- double [FcAB](#)
true hybrid states only
- double [FA](#)
monomer A
- double [FB](#)
monomer B

15.46.2.2 struct vrna_dimer_conc_s

Data structure for concentration dependency computations.

Data Fields

- double [A0](#)
start concentration A
- double [B0](#)
start concentration B
- double [ABc](#)
End concentration AB.

15.46.3 Function Documentation

15.46.3.1 vrna_dimer_pf_t vrna_pf_dimer (vrna_fold_compound_t * vc, char * structure)

```
#include <ViennaRNA/part_func_co.h>
```

Calculate partition function and base pair probabilities of nucleic acid/nucleic acid dimers.

This is the cofold partition function folding.

See also

[vrna_fold_compound\(\)](#) for how to retrieve the necessary data structure

Parameters

<i>vc</i>	the fold compound data structure
<i>structure</i>	Will hold the structure or constraints

Returns

vrna_dimer_pf_t structure containing a set of energies needed for concentration computations.

SWIG Wrapper Notes This function is attached as method **pf_dimer()** to objects of type *fold_compound*

15.46.3.2 void vrna_pf_dimer_probs (double FAB, double FA, double FB, vrna_plist_t * prAB, const vrna_plist_t * prA, const vrna_plist_t * prB, int Alength, const vrna_exp_param_t * exp_params)

```
#include <ViennaRNA/part_func_co.h>
```

Compute Boltzmann probabilities of dimerization without homodimers.

Given the pair probabilities and free energies (in the null model) for a dimer AB and the two constituent monomers A and B, compute the conditional pair probabilities given that a dimer AB actually forms. Null model pair probabilities are given as a list as produced by [vrna_plist_from_probs\(\)](#), the dimer probabilities 'prAB' are modified in place.

Parameters

<i>FAB</i>	free energy of dimer AB
<i>FA</i>	free energy of monomer A
<i>FB</i>	free energy of monomer B
<i>prAB</i>	pair probabilities for dimer
<i>prA</i>	pair probabilities monomer
<i>prB</i>	pair probabilities monomer
<i>Alength</i>	Length of molecule A
<i>exp_params</i>	The precomputed Boltzmann factors

15.46.3.3 `vrna_dimer_conc_t* vrna_pf_dimer_concentrations (double FcAB, double FcAA, double FcBB, double FEA, double FEB, const double * startconc, const vrna_exp_param_t * exp_params)`

```
#include <ViennaRNA/part_func_co.h>
```

Given two start monomer concentrations a and b, compute the concentrations in thermodynamic equilibrium of all dimers and the monomers.

This function takes an array 'startconc' of input concentrations with alternating entries for the initial concentrations of molecules A and B (terminated by two zeroes), then computes the resulting equilibrium concentrations from the free energies for the dimers. Dimer free energies should be the dimer-only free energies, i.e. the *FcAB* entries from the `vrna_dimer_pf_t` struct.

Parameters

<i>FcAB</i>	Free energy of AB dimer (<i>FcAB</i> entry)
<i>FcAA</i>	Free energy of AA dimer (<i>FcAB</i> entry)
<i>FcBB</i>	Free energy of BB dimer (<i>FcAB</i> entry)
<i>FEA</i>	Free energy of monomer A
<i>FEB</i>	Free energy of monomer B
<i>startconc</i>	List of start concentrations [a0],[b0],[a1],[b1],...,[an],[bn],[0],[0]
<i>exp_params</i>	The precomputed Boltzmann factors

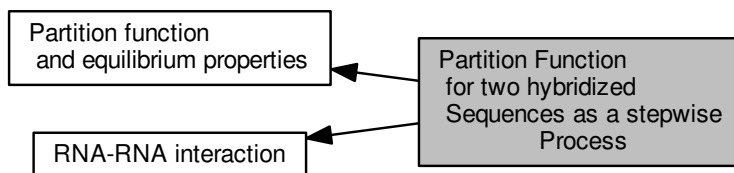
Returns

`vrna_dimer_conc_t` array containing the equilibrium energies and start concentrations

15.47 Partition Function for two hybridized Sequences as a stepwise Process

RNA-RNA interaction as a stepwise process.

Collaboration diagram for Partition Function for two hybridized Sequences as a stepwise Process:



Functions

- `pu_contrib * pf_unstru (char *sequence, int max_w)`
Calculate the partition function over all unpaired regions of a maximal length.
- `interact * pf_interact (const char *s1, const char *s2, pu_contrib *p_c, pu_contrib *p_c2, int max_w, char *cstruc, int incr3, int incr5)`
Calculates the probability of a local interaction between two sequences.
- `void free_interact (interact *pin)`
Frees the output of function `pf_interact()`.
- `void free_pu_contrib_struct (pu_contrib *pu)`
Frees the output of function `pf_unstru()`.

15.47.1 Detailed Description

RNA-RNA interaction as a stepwise process.

In this approach to cofolding the interaction between two RNA molecules is seen as a stepwise process. In a first step, the target molecule has to adopt a structure in which a binding site is accessible. In a second step, the ligand molecule will hybridize with a region accessible to an interaction. Consequently the algorithm is designed as a two step process: The first step is the calculation of the probability that a region within the target is unpaired, or equivalently, the calculation of the free energy needed to expose a region. In the second step we compute the free energy of an interaction for every possible binding site.

15.47.2 Function Documentation

15.47.2.1 `pu_contrib* pf_unstru (char * sequence, int max_w)`

```
#include <ViennaRNA/part_func_up.h>
```

Calculate the partition function over all unpaired regions of a maximal length.

You have to call function `pf_fold()` providing the same sequence before calling `pf_unstru()`. If you want to calculate unpaired regions for a constrained structure, set variable 'structure' in function '`pf_fold()`' to the constrain string. It returns a `pu_contrib` struct containing four arrays of dimension $[i = 1 \text{ to } \text{length}(\text{sequence})][j = 0 \text{ to } u-1]$ containing all possible contributions to the probabilities of unpaired regions of maximum length u . Each array in `pu_contrib` contains one of the contributions to the total probability of being unpaired: The probability of being unpaired within an exterior loop is in array `pu_contrib->E`, the probability of being unpaired within a hairpin loop is in array `pu_contrib->H`, the probability of being unpaired within an interior loop is in array `pu_contrib->I` and probability of being unpaired within a multi-loop is in array `pu_contrib->M`. The total probability of being unpaired is the sum of the four arrays of `pu_contrib`.

This function frees everything allocated automatically. To free the output structure call `free_pu_contrib()`.

Parameters

<i>sequence</i>	
<i>max_w</i>	

Returns

15.47.2.2 `interact* pf_interact (const char * s1, const char * s2, pu_contrib * p_c, pu_contrib * p_c2, int max_w, char * cstruc, int incr3, int incr5)`

```
#include <ViennaRNA/part_func_up.h>
```

Calculates the probability of a local interaction between two sequences.

The function considers the probability that the region of interaction is unpaired within 's1' and 's2'. The longer sequence has to be given as 's1'. The shorter sequence has to be given as 's2'. Function `pf_unstru()` has to be called for 's1' and 's2', where the probabilities of being unpaired have to be given in 'p_c' and 'p_c2', respectively. If you do not want to include the probabilities of being unpaired for 's2' set 'p_c2' to NULL. If variable 'cstruc' is not NULL, constrained folding is done: The available constrains for intermolecular interaction are: '.' (no constrain), 'x' (the base has no intermolecular interaction) and '|' (the corresponding base has to be paired intermolecularly). The parameter 'w' determines the maximal length of the interaction. The parameters 'incr5' and 'incr3' allows inclusion of unpaired residues left ('incr5') and right ('incr3') of the region of interaction in 's1'. If the 'incr' options are used, function `pf_unstru()` has to be called with $w = w + \text{incr5} + \text{incr3}$ for the longer sequence 's1'.

It returns a structure of type `interact` which contains the probability of the best local interaction including residue i in P_i and the minimum free energy in G_i , where i is the position in sequence 's1'. The member G_{ikjl} of structure `interact` is the best interaction between region $[k,i]$ $k < i$ in longer sequence 's1' and region $[j,l]$ $j < l$ in 's2'. G_{ikjl_wo} is G_{ikjl} without the probability of being unpaired.

Use `free_interact()` to free the returned structure, all other stuff is freed inside `pf_interact()`.

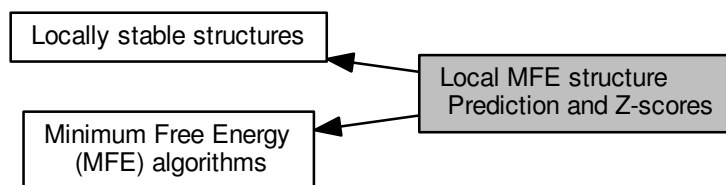
Parameters

<i>s1</i>	
<i>s2</i>	
<i>p_c</i>	
<i>p_c2</i>	
<i>max_w</i>	
<i>cstruc</i>	
<i>incr3</i>	
<i>incr5</i>	

Returns

15.48 Local MFE structure Prediction and Z-scores

Collaboration diagram for Local MFE structure Prediction and Z-scores:



Functions

- float [vrna_Lfold](#) (const char *string, int window_size, FILE *file)
Local MFE prediction using a sliding window approach (simplified interface)
- float [vrna_Lfoldz](#) (const char *string, int window_size, double min_z, FILE *file)
Local MFE prediction using a sliding window approach with z-score cut-off (simplified interface)
- float [Lfold](#) (const char *string, char *structure, int maxdist)
The local analog to [fold\(\)](#).
- float [Lfoldz](#) (const char *string, char *structure, int maxdist, int zsc, double min_z)
- float [vrna_mfe_window](#) ([vrna_fold_compound_t](#) *vc, FILE *file)
Local MFE prediction using a sliding window approach.
- float [vrna_mfe_window_zscore](#) ([vrna_fold_compound_t](#) *vc, double min_z, FILE *file)
Local MFE prediction using a sliding window approach (with z-score cut-off)

15.48.1 Detailed Description

15.48.2 Function Documentation

15.48.2.1 float [vrna_Lfold](#) (const char * *string*, int *window_size*, FILE * *file*)

```
#include <ViennaRNA/Lfold.h>
```

Local MFE prediction using a sliding window approach (simplified interface)

This simplified interface to [vrna_mfe_window\(\)](#) computes the MFE and locally optimal secondary structure using default options. Structures are predicted using a sliding window approach, where base pairs may not span outside the window. Memory required for dynamic programming (DP) matrices will be allocated and free'd on-the-fly. Hence, after return of this function, the recursively filled matrices are not available any more for any post-processing.

Note

In case you want to use the filled DP matrices for any subsequent post-processing step, or you require other conditions than specified by the default model details, use [vrna_mfe_window\(\)](#), and the data structure [vrna_fold_compound_t](#) instead.

See also

[vrna_mfe_window\(\)](#), [vrna_Lfoldz\(\)](#), [vrna_mfe_window_zscore\(\)](#), [vrna_fold_compound\(\)](#), [vrna_fold_compound_t](#)

Parameters

<i>string</i>	The nucleic acid sequence
<i>window_size</i>	The window size for locally optimal structures
<i>file</i>	The output file handle where predictions are written to (if NULL, output is written to stdout)

15.48.2.2 `float vrna_Lfoldz (const char * string, int window_size, double min_z, FILE * file)`

```
#include <ViennaRNA/Lfold.h>
```

Local MFE prediction using a sliding window approach with z-score cut-off (simplified interface)

This simplified interface to [vrna_mfe_window_zscore\(\)](#) computes the MFE and locally optimal secondary structure using default options. Structures are predicted using a sliding window approach, where base pairs may not span outside the window. Memory required for dynamic programming (DP) matrices will be allocated and free'd on-the-fly. Hence, after return of this function, the recursively filled matrices are not available any more for any post-processing. This function is the z-score version of [vrna_Lfold\(\)](#), i.e. only predictions above a certain z-score cut-off value are printed.

Note

In case you want to use the filled DP matrices for any subsequent post-processing step, or you require other conditions than specified by the default model details, use [vrna_mfe_window\(\)](#), and the data structure [vrna_fold_compound_t](#) instead.

See also

[vrna_mfe_window_zscore\(\)](#), [vrna_Lfold\(\)](#), [vrna_mfe_window\(\)](#), [vrna_fold_compound\(\)](#), [vrna_fold_compound_t](#)

Parameters

<i>string</i>	The nucleic acid sequence
<i>window_size</i>	The window size for locally optimal structures
<i>min_z</i>	The minimal z-score for a predicted structure to appear in the output
<i>file</i>	The output file handle where predictions are written to (if NULL, output is written to stdout)

15.48.2.3 `float Lfold (const char * string, char * structure, int maxdist)`

```
#include <ViennaRNA/Lfold.h>
```

The local analog to [fold\(\)](#).

Computes the minimum free energy structure including only base pairs with a span smaller than 'maxdist'

Deprecated Use [vrna_mfe_window\(\)](#) instead!

15.48.2.4 float Lfoldz (const char * *string*, char * *structure*, int *maxdist*, int *zsc*, double *min_z*)

```
#include <ViennaRNA/Lfold.h>
```

Deprecated Use `vrna_mfe_window_zscore()` instead!

15.48.2.5 float vrna_mfe_window (vrna_fold_compound_t * *vc*, FILE * *file*)

```
#include <ViennaRNA/mfe.h>
```

Local MFE prediction using a sliding window approach.

Computes minimum free energy structures using a sliding window approach, where base pairs may not span outside the window. In contrast to `vrna_mfe()`, where a maximum base pair span may be set using the `vrna_md_t.max_bp_span` attribute and one globally optimal structure is predicted, this function uses a sliding window to retrieve all locally optimal structures within each window. The size of the sliding window is set in the `vrna_md_t.window_size` attribute, prior to the retrieval of the `vrna_fold_compound_t` using `vrna_fold_compound()` with option `VRNA_OPTION_WINDOW`

The predicted structures are written on-the-fly, either to stdout, if a NULL pointer is passed as file parameter, or to the corresponding filehandle.

See also

`vrna_fold_compound()`, `vrna_mfe_window_zscore()`, `vrna_mfe()`, `vrna_Lfold()`, `vrna_Lfoldz()`, `VRNA_OPTION_WINDOW`, `vrna_md_t.max_bp_span`, `vrna_md_t.window_size`

Parameters

<i>vc</i>	The <code>vrna_fold_compound_t</code> with preallocated memory for the DP matrices
<i>file</i>	The output file handle where predictions are written to (maybe NULL)

SWIG Wrapper Notes This function is attached as method `mfe_window()` to objects of type `fold_compound`

15.48.2.6 float vrna_mfe_window_zscore (vrna_fold_compound_t * *vc*, double *min_z*, FILE * *file*)

```
#include <ViennaRNA/mfe.h>
```

Local MFE prediction using a sliding window approach (with z-score cut-off)

Computes minimum free energy structures using a sliding window approach, where base pairs may not span outside the window. This function is the z-score version of `vrna_mfe_window()`, i.e. only predictions above a certain z-score cut-off value are printed. As for `vrna_mfe_window()`, the size of the sliding window is set in the `vrna_md_t.window_size` attribute, prior to the retrieval of the `vrna_fold_compound_t` using `vrna_fold_compound()` with option `VRNA_OPTION_WINDOW`.

The predicted structures are written on-the-fly, either to stdout, if a NULL pointer is passed as file parameter, or to the corresponding filehandle.

See also

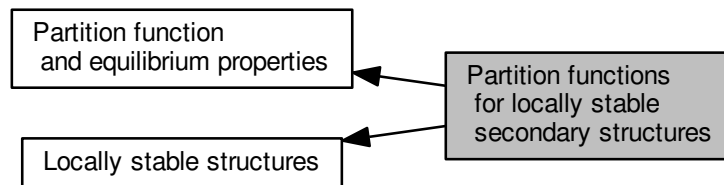
[vrna_fold_compound\(\)](#), [vrna_mfe_window_zscore\(\)](#), [vrna_mfe\(\)](#), [vrna_Lfold\(\)](#), [vrna_Lfoldz\(\)](#), [VRNA_OPTI←
ON_WINDOW](#), [vrna_md_t.max_bp_span](#), [vrna_md_t.window_size](#)

Parameters

<i>vc</i>	The vrna_fold_compound_t with preallocated memory for the DP matrices
<i>min_z</i>	The minimal z-score for a predicted structure to appear in the output
<i>file</i>	The output file handle where predictions are written to (maybe NULL)

15.49 Partition functions for locally stable secondary structures

Collaboration diagram for Partition functions for locally stable secondary structures:



Functions

- void `update_pf_paramsLP` (int length)
- `plist * pfl_fold` (char *sequence, int winSize, int pairSize, float cutoffb, double **pU, `plist **dpp2`, FILE *pUfp, FILE *spup)
Compute partition functions for locally stable secondary structures.
- `plist * pfl_fold_par` (char *sequence, int winSize, int pairSize, float cutoffb, double **pU, `plist **dpp2`, FILE *pUfp, FILE *spup, `vrna_exp_param_t` *parameters)
Compute partition functions for locally stable secondary structures.
- void `putoutpU_prob` (double **pU, int length, int ulength, FILE *fp, int energies)
Writes the unpaired probabilities (pU) or opening energies into a file.
- void `putoutpU_prob_bin` (double **pU, int length, int ulength, FILE *fp, int energies)
Writes the unpaired probabilities (pU) or opening energies into a binary file.

15.49.1 Detailed Description

15.49.2 Function Documentation

15.49.2.1 void update_pf_paramsLP (int length)

```
#include <ViennaRNA/LPfold.h>
```

Parameters

length	
--------	--

15.49.2.2 `plist* pfl_fold` (char * sequence, int winSize, int pairSize, float cutoffb, double ** pU, `plist ** dpp2`, FILE * pUfp, FILE * spup)

```
#include <ViennaRNA/LPfold.h>
```

Compute partition functions for locally stable secondary structures.

`pfl_fold` computes partition functions for every window of size '`winSize`' possible in a RNA molecule, allowing only pairs with a span smaller than '`pairSize`'. It returns the mean pair probabilities averaged over all windows containing the pair in '`pl`'. '`winSize`' should always be \geq '`pairSize`'. Note that in contrast to `Lfold()`, bases outside of the window do not influence the structure at all. Only probabilities higher than '`cutoffb`' are kept.

If '`pU`' is supplied (i.e. is not the NULL pointer), `pfl_fold()` will also compute the mean probability that regions of length '`u`' and smaller are unpaired. The parameter '`u`' is supplied in '`pup[0][0]`'. On return the '`pup`' array will contain these probabilities, with the entry on '`pup[x][y]`' containing the mean probability that `x` and the `y-1` preceding bases are unpaired. The '`pU`' array needs to be large enough to hold `n+1 float*` entries, where `n` is the sequence length.

If an array `dpp2` is supplied, the probability of base pair (`i,j`) given that there already exists a base pair (`i+1,j-1`) is also computed and saved in this array. If `pUfp` is given (i.e. not NULL), `pU` is not saved but put out immediately. If `spup` is given (i.e. is not NULL), the pair probabilities in `pl` are not saved but put out immediately.

Parameters

<i>sequence</i>	RNA sequence
<i>winSize</i>	size of the window
<i>pairSize</i>	maximum size of base pair
<i>cutoffb</i>	cutoffb for base pairs
<i>pU</i>	array holding all unpaired probabilities
<i>dpp2</i>	array of dependent pair probabilities
<i>pUfp</i>	file pointer for pU
<i>spup</i>	file pointer for pair probabilities

Returns

list of pair probabilities

15.49.2.3 `void putoutpU_prob (double ** pU, int length, int ulength, FILE * fp, int energies)`

```
#include <ViennaRNA/LPfold.h>
```

Writes the unpaired probabilities (`pU`) or opening energies into a file.

Can write either the unpaired probabilities (accessibilities) `pU` or the opening energies $-\log(pU)kT$ into a file

Parameters

<i>pU</i>	pair probabilities
<i>length</i>	length of RNA sequence
<i>ulength</i>	maximum length of unpaired stretch
<i>fp</i>	file pointer of destination file
<i>energies</i>	switch to put out as opening energies

15.49.2.4 `void putoutpU_prob_bin (double ** pU, int length, int ulength, FILE * fp, int energies)`

```
#include <ViennaRNA/LPfold.h>
```

Writes the unpaired probabilities (pU) or opening energies into a binary file.

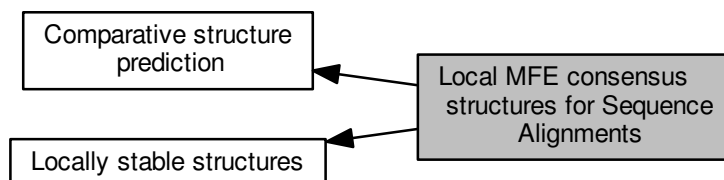
Can write either the unpaired probabilities (accessibilities) pU or the opening energies $-\log(pU)kT$ into a file

Parameters

<i>pU</i>	pair probabilities
<i>length</i>	length of RNA sequence
<i>ulength</i>	maximum length of unpaired stretch
<i>fp</i>	file pointer of destination file
<i>energies</i>	switch to put out as opening energies

15.50 Local MFE consensus structures for Sequence Alignments

Collaboration diagram for Local MFE consensus structures for Sequence Alignments:



Functions

- float [aliLfold](#) (const char **strings, char *structure, int maxdist)

15.50.1 Detailed Description

15.50.2 Function Documentation

15.50.2.1 float aliLfold (const char ** *strings*, char * *structure*, int *maxdist*)

```
#include <ViennaRNA/Lfold.h>
```

Parameters

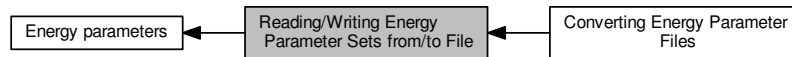
<i>strings</i>	
<i>structure</i>	
<i>maxdist</i>	

Returns

15.51 Reading/Writing Energy Parameter Sets from/to File

Read and Write energy parameter sets from and to text files.

Collaboration diagram for Reading/Writing Energy Parameter Sets from/to File:



Modules

- [Converting Energy Parameter Files](#)
Convert energy parameter files into the latest format.

Functions

- void [read_parameter_file](#) (const char fname[])
Read energy parameters from a file.
- void [write_parameter_file](#) (const char fname[])
Write energy parameters to a file.

15.51.1 Detailed Description

Read and Write energy parameter sets from and to text files.

A default set of parameters, identical to the one described in [14] and [19], is compiled into the library.

15.51.2 Function Documentation

15.51.2.1 void read_parameter_file (const char fname[])

```
#include <ViennaRNA/read_epars.h>
```

Read energy parameters from a file.

Parameters

<i>fname</i>	The path to the file containing the energy parameters
--------------	-------------------------------------------------------

15.51.2.2 void write_parameter_file (const char *fname*[])

```
#include <ViennaRNA/read_epars.h>
```

Write energy parameters to a file.

Parameters

<i>fname</i>	A filename (path) for the file where the current energy parameters will be written to
--------------	---------------------------------------------------------------------------------------

15.52 Converting Energy Parameter Files

Convert energy parameter files into the latest format.

Collaboration diagram for Converting Energy Parameter Files:



Files

- file [1.8.4_epars.h](#)
Free energy parameters for parameter file conversion.
- file [1.8.4_intloops.h](#)
Free energy parameters for interior loop contributions needed by the parameter file conversion functions.

Macros

- `#define VRNA_CONVERT_OUTPUT_ALL 1U`
- `#define VRNA_CONVERT_OUTPUT_HP 2U`
- `#define VRNA_CONVERT_OUTPUT_STACK 4U`
- `#define VRNA_CONVERT_OUTPUT_MM_HP 8U`
- `#define VRNA_CONVERT_OUTPUT_MM_INT 16U`
- `#define VRNA_CONVERT_OUTPUT_MM_INT_1N 32U`
- `#define VRNA_CONVERT_OUTPUT_MM_INT_23 64U`
- `#define VRNA_CONVERT_OUTPUT_MM_MULTI 128U`
- `#define VRNA_CONVERT_OUTPUT_MM_EXT 256U`
- `#define VRNA_CONVERT_OUTPUT_DANGLE5 512U`
- `#define VRNA_CONVERT_OUTPUT_DANGLE3 1024U`
- `#define VRNA_CONVERT_OUTPUT_INT_11 2048U`
- `#define VRNA_CONVERT_OUTPUT_INT_21 4096U`
- `#define VRNA_CONVERT_OUTPUT_INT_22 8192U`
- `#define VRNA_CONVERT_OUTPUT_BULGE 16384U`
- `#define VRNA_CONVERT_OUTPUT_INT 32768U`
- `#define VRNA_CONVERT_OUTPUT_ML 65536U`
- `#define VRNA_CONVERT_OUTPUT_MISC 131072U`
- `#define VRNA_CONVERT_OUTPUT_SPECIAL_HP 262144U`
- `#define VRNA_CONVERT_OUTPUT_VANILLA 524288U`
- `#define VRNA_CONVERT_OUTPUT_NINIO 1048576U`
- `#define VRNA_CONVERT_OUTPUT_DUMP 2097152U`

Functions

- void `convert_parameter_file` (const char *iname, const char *oname, unsigned int options)

15.52.1 Detailed Description

Convert energy parameter files into the latest format.

To preserve some backward compatibility the RNAlib also provides functions to convert energy parameter files from the format used in version 1.4-1.8 into the new format used since version 2.0

15.52.2 Macro Definition Documentation

15.52.2.1 `#define VRNA_CONVERT_OUTPUT_ALL 1U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate printing of a complete parameter set

15.52.2.2 `#define VRNA_CONVERT_OUTPUT_HP 2U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate printing of hairpin contributions

15.52.2.3 `#define VRNA_CONVERT_OUTPUT_STACK 4U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate printing of base pair stack contributions

15.52.2.4 `#define VRNA_CONVERT_OUTPUT_MM_HP 8U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate printing of hairpin mismatch contribution

15.52.2.5 `#define VRNA_CONVERT_OUTPUT_MM_INT 16U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate printing of interior loop mismatch contribution

15.52.2.6 `#define VRNA_CONVERT_OUTPUT_MM_INT_1N 32U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate printing of 1:n interior loop mismatch contribution

15.52.2.7 `#define VRNA_CONVERT_OUTPUT_MM_INT_23 64U`

`#include <ViennaRNA/convert_epars.h>`

Flag to indicate printing of 2:3 interior loop mismatch contribution

15.52.2.8 `#define VRNA_CONVERT_OUTPUT_MM_MULTI 128U`

`#include <ViennaRNA/convert_epars.h>`

Flag to indicate printing of multi loop mismatch contribution

15.52.2.9 `#define VRNA_CONVERT_OUTPUT_MM_EXT 256U`

`#include <ViennaRNA/convert_epars.h>`

Flag to indicate printing of exterior loop mismatch contribution

15.52.2.10 `#define VRNA_CONVERT_OUTPUT_DANGLE5 512U`

`#include <ViennaRNA/convert_epars.h>`

Flag to indicate printing of 5' dangle contribution

15.52.2.11 `#define VRNA_CONVERT_OUTPUT_DANGLE3 1024U`

`#include <ViennaRNA/convert_epars.h>`

Flag to indicate printing of 3' dangle contribution

15.52.2.12 `#define VRNA_CONVERT_OUTPUT_INT_11 2048U`

`#include <ViennaRNA/convert_epars.h>`

Flag to indicate printing of 1:1 interior loop contribution

15.52.2.13 `#define VRNA_CONVERT_OUTPUT_INT_21 4096U`

`#include <ViennaRNA/convert_epars.h>`

Flag to indicate printing of 2:1 interior loop contribution

15.52.2.14 `#define VRNA_CONVERT_OUTPUT_INT_22 8192U`

`#include <ViennaRNA/convert_epars.h>`

Flag to indicate printing of 2:2 interior loop contribution

15.52.2.15 `#define VRNA_CONVERT_OUTPUT_BULGE 16384U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate printing of bulge loop contribution

15.52.2.16 `#define VRNA_CONVERT_OUTPUT_INT 32768U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate printing of interior loop contribution

15.52.2.17 `#define VRNA_CONVERT_OUTPUT_ML 65536U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate printing of multi loop contribution

15.52.2.18 `#define VRNA_CONVERT_OUTPUT_MISC 131072U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate printing of misc contributions (such as terminalAU)

15.52.2.19 `#define VRNA_CONVERT_OUTPUT_SPECIAL_HP 262144U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate printing of special hairpin contributions (tri-, tetra-, hexa-loops)

15.52.2.20 `#define VRNA_CONVERT_OUTPUT_VANILLA 524288U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate printing of given parameters only

Note

This option overrides all other output options, except `VRNA_CONVERT_OUTPUT_DUMP` !

15.52.2.21 `#define VRNA_CONVERT_OUTPUT_NINIO 1048576U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate printing of interior loop asymmetry contribution

15.52.2.22 `#define VRNA_CONVERT_OUTPUT_DUMP 2097152U`

```
#include <ViennaRNA/convert_epars.h>
```

Flag to indicate dumping the energy contributions from the library instead of an input file

15.52.3 Function Documentation

15.52.3.1 `void convert_parameter_file (const char * iname, const char * oname, unsigned int options)`

```
#include <ViennaRNA/convert_epars.h>
```

Convert/dump a Vienna 1.8.4 formatted energy parameter file

The options argument allows one to control the different output modes.

Currently available options are:

```
VRNA_CONVERT_OUTPUT_ALL, VRNA_CONVERT_OUTPUT_HP, VRNA_CONVERT_OUTPUT_STACK
VRNA_CONVERT_OUTPUT_MM_HP, VRNA_CONVERT_OUTPUT_MM_INT, VRNA_CONVERT_OUTPUT_↵
MM_INT_1N
VRNA_CONVERT_OUTPUT_MM_INT_23, VRNA_CONVERT_OUTPUT_MM_MULTI, VRNA_CONVERT_OUT↵
PUT_MM_EXT
VRNA_CONVERT_OUTPUT_DANGLE5, VRNA_CONVERT_OUTPUT_DANGLE3, VRNA_CONVERT_OUTPU↵
T_INT_11
VRNA_CONVERT_OUTPUT_INT_21, VRNA_CONVERT_OUTPUT_INT_22, VRNA_CONVERT_OUTPUT_BU↵
LGE
VRNA_CONVERT_OUTPUT_INT, VRNA_CONVERT_OUTPUT_ML, VRNA_CONVERT_OUTPUT_MISC
VRNA_CONVERT_OUTPUT_SPECIAL_HP, VRNA_CONVERT_OUTPUT_VANILLA, VRNA_CONVERT_OUT↵
PUT_NINIO
VRNA_CONVERT_OUTPUT_DUMP
```

The defined options are fine for bitwise compare- and assignment-operations, e. g.: pass a collection of options as a single value like this:

```
convert_parameter_file(ifile, ofile, option_1 | option_2 | option_n)
```

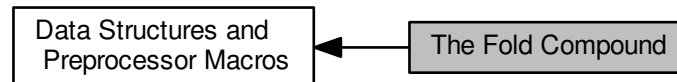
Parameters

<i>iname</i>	The input file name (If NULL input is read from stdin)
<i>oname</i>	The output file name (If NULL output is written to stdout)
<i>options</i>	The options (as described above)

15.53 The Fold Compound

This module provides interfaces that deal with the most basic data structure used in structure predicting and energy evaluating function of the RNAlib.

Collaboration diagram for The Fold Compound:



Data Structures

- struct [vrna_fc_s](#)

The most basic data structure required by many functions throughout the RNAlib. [More...](#)

Macros

- #define [VRNA_STATUS_MFE_PRE](#) (unsigned char)1
Status message indicating that MFE computations are about to begin.
- #define [VRNA_STATUS_MFE_POST](#) (unsigned char)2
Status message indicating that MFE computations are finished.
- #define [VRNA_STATUS_PF_PRE](#) (unsigned char)3
Status message indicating that Partition function computations are about to begin.
- #define [VRNA_STATUS_PF_POST](#) (unsigned char)4
Status message indicating that Partition function computations are finished.
- #define [VRNA_OPTION_DEFAULT](#) 0U
Option flag to specify default settings/requirements.
- #define [VRNA_OPTION_MFE](#) 1U
Option flag to specify requirement of Minimum Free Energy (MFE) DP matrices and corresponding set of energy parameters.
- #define [VRNA_OPTION_PF](#) 2U
Option flag to specify requirement of Partition Function (PF) DP matrices and corresponding set of Boltzmann factors.
- #define [VRNA_OPTION_HYBRID](#) 4U
Option flag to specify requirement of dimer DP matrices.
- #define [VRNA_OPTION_EVAL_ONLY](#) 8U
Option flag to specify that neither MFE, nor PF DP matrices are required.
- #define [VRNA_OPTION_WINDOW](#) 16U
Option flag to specify requirement of DP matrices for local folding approaches.

Typedefs

- typedef struct [vrna_fc_s](#) [vrna_fold_compound_t](#)
Typename for the fold_compound data structure [vrna_fc_s](#).
- typedef void([vrna_callback_free_auxdata](#)) (void *data)
Callback to free memory allocated for auxiliary user-provided data.
- typedef void([vrna_callback_recursion_status](#)) (unsigned char status, void *data)
Callback to perform specific user-defined actions before, or after recursive computations.

Enumerations

Functions

- [vrna_fold_compound_t](#) * [vrna_fold_compound](#) (const char *sequence, [vrna_md_t](#) *md_p, unsigned int options)
Retrieve a [vrna_fold_compound_t](#) data structure for single sequences and hybridizing sequences.
- [vrna_fold_compound_t](#) * [vrna_fold_compound_comparative](#) (const char **sequences, [vrna_md_t](#) *md_p, unsigned int options)
Retrieve a [vrna_fold_compound_t](#) data structure for sequence alignments.
- void [vrna_fold_compound_free](#) ([vrna_fold_compound_t](#) *vc)
Free memory occupied by a [vrna_fold_compound_t](#).
- void [vrna_fold_compound_add_auxdata](#) ([vrna_fold_compound_t](#) *vc, void *data, [vrna_callback_free_auxdata](#) *f)
Add auxiliary data to the [vrna_fold_compound_t](#).
- void [vrna_fold_compound_add_callback](#) ([vrna_fold_compound_t](#) *vc, [vrna_callback_recursion_status](#) *f)
Add a recursion status callback to the [vrna_fold_compound_t](#).

15.53.1 Detailed Description

This module provides interfaces that deal with the most basic data structure used in structure predicting and energy evaluating function of the RNAlib.

Throughout the entire RNAlib, the [vrna_fold_compound_t](#), is used to group information and data that is required for structure prediction and energy evaluation. Here, you'll find interface functions to create, modify, and delete [vrna_fold_compound_t](#) data structures.

15.53.2 Data Structure Documentation

15.53.2.1 struct [vrna_fc_s](#)

The most basic data structure required by many functions throughout the RNAlib.

Note

Please read the documentation of this data structure carefully! Some attributes are only available for specific types this data structure can adopt.

Warning

Reading/Writing from/to attributes that are not within the scope of the current type usually result in undefined behavior!

See also

[vrna_fold_compound_t.type](#), [vrna_fold_compound\(\)](#), [vrna_fold_compound_comparative\(\)](#), [vrna_fold_compound_free\(\)](#), [VRNA_FC_TYPE_SINGLE](#), [VRNA_FC_TYPE_COMPARATIVE](#)

SWIG Wrapper Notes This data structure is wrapped as an object **fold_compound** with several related functions attached as methods.

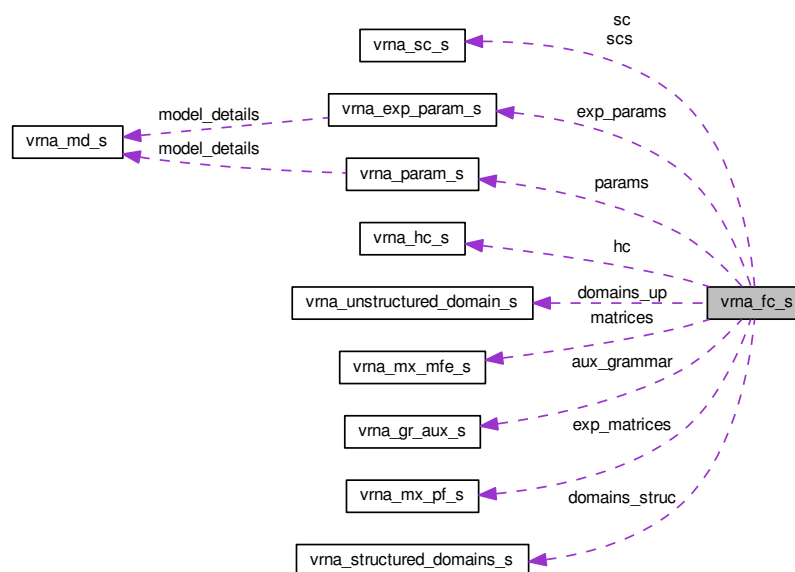
A new **fold_compound** can be obtained by calling one of its constructors:

- *fold_compound(seq)* – Initialize with a single sequence, or two concatenated sequences separated by an ampersand character '&' (for cofolding)
- *fold_compound(aln)* – Initialize with a sequence alignment *aln* stored as a list of sequences (with gap characters)

The resulting object has a list of attached methods which in most cases directly correspond to functions that mainly operate on the corresponding C data structure:

- *type()* – Get the type of the *fold_compound* (See [vrna_fc_type_e](#))
- *length()* – Get the length of the sequence(s) or alignment stored within the *fold_compound*

Collaboration diagram for `vrna_fc_s`:



Data Fields

Common data fields

- [vrna_fc_type_e](#) type
The type of the [vrna_fold_compound_t](#).
- unsigned int [length](#)
The length of the sequence (or sequence alignment)
- int [cutpoint](#)
The position of the (cofold) cutpoint within the provided sequence. If there is no cutpoint, this field will be set to -1.
- [vrna_hc_t](#) * [hc](#)
The hard constraints data structure used for structure prediction.
- [vrna_mx_mfe_t](#) * [matrices](#)
The MFE DP matrices.
- [vrna_mx_pf_t](#) * [exp_matrices](#)
The PF DP matrices.
- [vrna_param_t](#) * [params](#)
The precomputed free energy contributions for each type of loop.
- [vrna_exp_param_t](#) * [exp_params](#)
The precomputed free energy contributions as Boltzmann factors.
- int * [iindx](#)
DP matrix accessor.
- int * [jindx](#)
DP matrix accessor.

User-defined data fields

- [vrna_callback_recursion_status](#) * [stat_cb](#)
Recursion status callback (usually called just before, and after recursive computations in the library).
- void * [auxdata](#)
A pointer to auxiliary, user-defined data.
- [vrna_callback_free_auxdata](#) * [free_auxdata](#)
A callback to free auxiliary user data whenever the [fold_compound](#) itself is free'd.

Secondary Structure Decomposition (grammar) related data fields

- [vrna_sd_t](#) * [domains_struct](#)
Additional structured domains.
- [vrna_ud_t](#) * [domains_unstr](#)
Additional unstructured domains.
- [vrna_gr_aux_t](#) * [aux_grammar](#)

Data fields available for single/hybrid structure prediction

Data fields for consensus structure prediction

Additional data fields for Distance Class Partitioning

These data fields are typically populated with meaningful data only if used in the context of Distance Class Partitioning

- unsigned int [maxD1](#)
Maximum allowed base pair distance to first reference.
- unsigned int [maxD2](#)
Maximum allowed base pair distance to second reference.

- short * [reference_pt1](#)
A pairtable of the first reference structure.
- short * [reference_pt2](#)
A pairtable of the second reference structure.
- unsigned int * [referenceBPs1](#)
Matrix containing number of basepairs of reference structure1 in interval [i,j].
- unsigned int * [referenceBPs2](#)
Matrix containing number of basepairs of reference structure2 in interval [i,j].
- unsigned int * [bpdist](#)
Matrix containing base pair distance of reference structure 1 and 2 on interval [i,j].
- unsigned int * [mm1](#)
Maximum matching matrix, reference struct 1 disallowed.
- unsigned int * [mm2](#)
Maximum matching matrix, reference struct 2 disallowed.

Additional data fields for local folding

These data fields are typically populated with meaningful data only if used in the context of local folding

- int [window_size](#)
window size for local folding sliding window approach
- char ** [ptype_local](#)
Pair type array (for local folding)

15.53.2.1.1 Field Documentation

15.53.2.1.1.1 [vrna_fc_type_e](#) [vrna_fc_s::type](#)

The type of the [vrna_fold_compound_t](#).

Currently possible values are [VRNA_FC_TYPE_SINGLE](#), and [VRNA_FC_TYPE_COMPARATIVE](#)

Warning

Do not edit this attribute, it will be automagically set by the corresponding `get()` methods for the [vrna_fold_compound_t](#). The value specified in this attribute dictates the set of other attributes to use within this data structure.

15.53.2.1.1.2 [vrna_callback_recursion_status*](#) [vrna_fc_s::stat_cb](#)

Recursion status callback (usually called just before, and after recursive computations in the library).

See also

[vrna_callback_recursion_status\(\)](#), [vrna_fold_compound_add_callback\(\)](#)

15.53.2.1.1.3 [void*](#) [vrna_fc_s::auxdata](#)

A pointer to auxiliary, user-defined data.

See also

[vrna_fold_compound_add_auxdata\(\)](#), [vrna_fold_compound_t.free_auxdata](#)

15.53.2.1.1.4 `vrna_callback_free_auxdata*` `vrna_fc_s::free_auxdata`

A callback to free auxiliary user data whenever the fold_compound itself is free'd.

See also

[vrna_fold_compound_t.auxdata](#), [vrna_callback_free_auxdata\(\)](#)

15.53.2.1.1.5 `char*` `vrna_fc_s::sequence`

The input sequence string.

Warning

Only available if

`type==VRNA_FC_TYPE_SINGLE`

15.53.2.1.1.6 `short*` `vrna_fc_s::sequence_encoding`

Numerical encoding of the input sequence.

See also

[vrna_sequence_encode\(\)](#)

Warning

Only available if

`type==VRNA_FC_TYPE_SINGLE`

15.53.2.1.1.7 `char*` `vrna_fc_s::ptype`

Pair type array.

Contains the numerical encoding of the pair type for each pair (i,j) used in MFE, Partition function and Evaluation computations.

Note

This array is always indexed via `jindx`, in contrast to previously different indexing between mfe and pf variants!

Warning

Only available if

`type==VRNA_FC_TYPE_SINGLE`

See also

[vrna_idx_col_wise\(\)](#), [vrna_ptypes\(\)](#)

15.53.2.1.1.8 `char* vrna_fc_s::ptype_pf_compat`

ptype array indexed via iidx

Deprecated This attribute will vanish in the future! It's meant for backward compatibility only!

Warning

Only available if

```
type==VRNA_FC_TYPE_SINGLE
```

15.53.2.1.1.9 `vrna_sc_t* vrna_fc_s::sc`

The soft constraints for usage in structure prediction and evaluation.

Warning

Only available if

```
type==VRNA_FC_TYPE_SINGLE
```

15.53.2.1.1.10 `char** vrna_fc_s::sequences`

The aligned sequences.

Note

The end of the alignment is indicated by a NULL pointer in the second dimension

Warning

Only available if

```
type==VRNA_FC_TYPE_COMPARATIVE
```

15.53.2.1.1.11 `unsigned int vrna_fc_s::n_seq`

The number of sequences in the alignment.

Warning

Only available if

```
type==VRNA_FC_TYPE_COMPARATIVE
```

15.53.2.1.1.12 `char* vrna_fc_s::cons_seq`

The consensus sequence of the aligned sequences.

Warning

Only available if

```
type==VRNA_FC_TYPE_COMPARATIVE
```

15.53.2.1.1.13 short* vrna_fc_s::S_cons

Numerical encoding of the consensus sequence.

Warning

Only available if

```
type==VRNA_FC_TYPE_COMPARATIVE
```

15.53.2.1.1.14 short vrna_fc_s::S**

Numerical encoding of the sequences in the alignment.

Warning

Only available if

```
type==VRNA_FC_TYPE_COMPARATIVE
```

15.53.2.1.1.15 short vrna_fc_s::S5**

S5[s][i] holds next base 5' of i in sequence s.

Warning

Only available if

```
type==VRNA_FC_TYPE_COMPARATIVE
```

15.53.2.1.1.16 short vrna_fc_s::S3**

S3[s][i] holds next base 3' of i in sequence s.

Warning

Only available if

```
type==VRNA_FC_TYPE_COMPARATIVE
```

15.53.2.1.1.17 int* vrna_fc_s::pscore

Precomputed array of pair types expressed as pairing scores.

Warning

Only available if

```
type==VRNA_FC_TYPE_COMPARATIVE
```

15.53.2.1.1.18 `short* vrna_fc_s::pscore_pf_compat`

Precomputed array of pair types expressed as pairing scores indexed via iindx.

Deprecated This attribute will vanish in the future!

Warning

Only available if

```
type==VRNA_FC_TYPE_COMPARATIVE
```

15.53.2.1.1.19 `vrna_sc_t** vrna_fc_s::scs`

A set of soft constraints (for each sequence in the alignment)

Warning

Only available if

```
type==VRNA_FC_TYPE_COMPARATIVE
```

15.53.3 Macro Definition Documentation

15.53.3.1 `#define VRNA_STATUS_MFE_PRE (unsigned char)1`

```
#include <ViennaRNA/data_structures.h>
```

Status message indicating that MFE computations are about to begin.

See also

[vrna_fold_compound_t.stat_cb](#), [vrna_callback_recursion_status\(\)](#), [vrna_mfe\(\)](#), [vrna_fold\(\)](#), [vrna_circfold\(\)](#), [vrna_alifold\(\)](#), [vrna_circalifold\(\)](#), [vrna_cofold\(\)](#)

15.53.3.2 `#define VRNA_STATUS_MFE_POST (unsigned char)2`

```
#include <ViennaRNA/data_structures.h>
```

Status message indicating that MFE computations are finished.

See also

[vrna_fold_compound_t.stat_cb](#), [vrna_callback_recursion_status\(\)](#), [vrna_mfe\(\)](#), [vrna_fold\(\)](#), [vrna_circfold\(\)](#), [vrna_alifold\(\)](#), [vrna_circalifold\(\)](#), [vrna_cofold\(\)](#)

15.53.3.3 #define VRNA_STATUS_PF_PRE (unsigned char)3

```
#include <ViennaRNA/data_structures.h>
```

Status message indicating that Partition function computations are about to begin.

See also

[vrna_fold_compound_t.stat_cb](#), [vrna_callback_recursion_status\(\)](#), [vrna_pf\(\)](#)

15.53.3.4 #define VRNA_STATUS_PF_POST (unsigned char)4

```
#include <ViennaRNA/data_structures.h>
```

Status message indicating that Partition function computations are finished.

See also

[vrna_fold_compound_t.stat_cb](#), [vrna_callback_recursion_status\(\)](#), [vrna_pf\(\)](#)

15.53.3.5 #define VRNA_OPTION_MFE 1U

```
#include <ViennaRNA/data_structures.h>
```

Option flag to specify requirement of Minimum Free Energy (MFE) DP matrices and corresponding set of energy parameters.

See also

[vrna_fold_compound\(\)](#), [vrna_fold_compound_comparative\(\)](#), [VRNA_OPTION_EVAL_ONLY](#)

15.53.3.6 #define VRNA_OPTION_PF 2U

```
#include <ViennaRNA/data_structures.h>
```

Option flag to specify requirement of Partition Function (PF) DP matrices and corresponding set of Boltzmann factors.

See also

[vrna_fold_compound\(\)](#), [vrna_fold_compound_comparative\(\)](#), [VRNA_OPTION_EVAL_ONLY](#)

15.53.3.7 `#define VRNA_OPTION_EVAL_ONLY 8U`

```
#include <ViennaRNA/data_structures.h>
```

Option flag to specify that neither MFE, nor PF DP matrices are required.

Use this flag in conjunction with `VRNA_OPTION_MFE`, and `VRNA_OPTION_PF` to save memory for a `vrna_fold_compound_t` obtained from `vrna_fold_compound()`, or `vrna_fold_compound_comparative()` in cases where only energy evaluation but no structure prediction is required.

See also

`vrna_fold_compound()`, `vrna_fold_compound_comparative()`, `vrna_eval_structure()`

15.53.4 Typedef Documentation

15.53.4.1 `typedef void(vrna_callback_free_auxdata)(void *data)`

```
#include <ViennaRNA/data_structures.h>
```

Callback to free memory allocated for auxiliary user-provided data.

This type of user-implemented function usually deletes auxiliary data structures. The user must take care to free all the memory occupied by the data structure passed.

Parameters

<i>data</i>	The data that needs to be free'd
-------------	----------------------------------

15.53.4.2 `typedef void(vrna_callback_recursion_status)(unsigned char status, void *data)`

```
#include <ViennaRNA/data_structures.h>
```

Callback to perform specific user-defined actions before, or after recursive computations.

See also

`VRNA_STATUS_MFE_PRE`, `VRNA_STATUS_MFE_POST`, `VRNA_STATUS_PF_PRE`, `VRNA_STATUS_PF_POST`

Parameters

<i>status</i>	The status indicator
<i>data</i>	The data structure that was assigned with <code>vrna_fold_compound_add_auxdata()</code>
<i>status</i>	The status indicator

15.53.5 Enumeration Type Documentation

15.53.5.1 enum `vrna_fc_type_e`

```
#include <ViennaRNA/data_structures.h>
```

An enumerator that is used to specify the type of a `vrna_fold_compound_t`.

Enumerator

`VRNA_FC_TYPE_SINGLE` Type is suitable for single, and hybridizing sequences

`VRNA_FC_TYPE_COMPARATIVE` Type is suitable for sequence alignments (consensus structure prediction)

15.53.6 Function Documentation

15.53.6.1 `vrna_fold_compound_t*` `vrna_fold_compound` (`const char *` *sequence*, `vrna_md_t *` *md_p*, unsigned int *options*)

```
#include <ViennaRNA/data_structures.h>
```

Retrieve a `vrna_fold_compound_t` data structure for single sequences and hybridizing sequences.

This function provides an easy interface to obtain a prefilled `vrna_fold_compound_t` by passing a single sequence, or two concatenated sequences as input. For the latter, sequences need to be separated by an '&' character like this:

```
char *sequence = "GGGG&CCCC";
```

The optional parameter `md_p` can be used to specify the model details for successive computations based on the content of the generated `vrna_fold_compound_t`. Passing NULL will instruct the function to use default model details. The third parameter `options` may be used to specify dynamic programming (DP) matrix requirements. Use the macros:

- `VRNA_OPTION_MFE`
- `VRNA_OPTION_PF`
- `VRNA_OPTION_WINDOW`
- `VRNA_OPTION_EVAL_ONLY`
- `VRNA_OPTION_DEFAULT`

to specify the required type of computations that will be performed with the `vrna_fold_compound_t`.

If you just need the folding compound serving as a container for your data, you can simply pass `VRNA_OPTION_DEFAULT` to the `option` parameter. This creates a `vrna_fold_compound_t` without DP matrices, thus saving memory. Subsequent calls of any structure prediction function will then take care of allocating the memory required for the DP matrices. If you only intend to evaluate structures instead of actually predicting them, you may use the `VRNA_OPTION_EVAL_ONLY` macro. This will seriously speedup the creation of the `vrna_fold_compound_t`.

Note

The sequence string must be uppercase, and should contain only RNA (resp. DNA) alphabet depending on what energy parameter set is used

See also

`vrna_fold_compound_free()`, `vrna_fold_compound_comparative()`, `vrna_md_t`, `VRNA_OPTION_MFE`, `VRNA_OPTION_PF`, `VRNA_OPTION_EVAL_ONLY`, `VRNA_OPTION_WINDOW`

Parameters

<i>sequence</i>	A single sequence, or two concatenated sequences seperated by an '&' character
<i>md_p</i>	An optional set of model details
<i>options</i>	The options for DP matrices memory allocation

Returns

A prefilled `vrna_fold_compound_t` that can be readily used for computations

15.53.6.2 `vrna_fold_compound_t* vrna_fold_compound_comparative (const char ** sequences, vrna_md_t * md_p, unsigned int options)`

```
#include <ViennaRNA/data_structures.h>
```

Retrieve a `vrna_fold_compound_t` data structure for sequence alignments.

This function provides an easy interface to obtain a prefilled `vrna_fold_compound_t` by passing an alignment of sequences.

The optional parameter `md_p` can be used to specify the model details for successive computations based on the content of the generated `vrna_fold_compound_t`. Passing NULL will instruct the function to use default model details. The third parameter `options` may be used to specify dynamic programming (DP) matrix requirements. Use the macros:

- `VRNA_OPTION_MFE`
- `VRNA_OPTION_PF`
- `VRNA_OPTION_EVAL_ONLY`
- `VRNA_OPTION_DEFAULT`

to specify the required type of computations that will be performed with the `vrna_fold_compound_t`.

If you just need the folding compound serving as a container for your data, you can simply pass `VRNA_OPTION_DEFAULT` to the `option` parameter. This creates a `vrna_fold_compound_t` without DP matrices, thus saving memory. Subsequent calls of any structure prediction function will then take care of allocating the memory required for the DP matrices. If you only intend to evaluate structures instead of actually predicting them, you may use the `VRNA_OPTION_EVAL_ONLY` macro. This will seriously speedup the creation of the `vrna_fold_compound_t`.

Note

The sequence strings must be uppercase, and should contain only RNA (resp. DNA) alphabet including gap characters depending on what energy parameter set is used.

See also

`vrna_fold_compound_free()`, `vrna_fold_compound()`, `vrna_md_t`, `VRNA_OPTION_MFE`, `VRNA_OPTION_`↵
`PF`, `VRNA_OPTION_EVAL_ONLY`, `read_clustal()`

Parameters

<i>sequences</i>	A sequence alignment including 'gap' characters
<i>md_p</i>	An optional set of model details
<i>options</i>	The options for DP matrices memory allocation

Returns

A prefilled `vrna_fold_compound_t` that can be readily used for computations

15.53.6.3 `void vrna_fold_compound_free (vrna_fold_compound_t * vc)`

```
#include <ViennaRNA/data_structures.h>
```

Free memory occupied by a `vrna_fold_compound_t`.

See also

[vrna_fold_compound\(\)](#), [vrna_fold_compound_comparative\(\)](#), [vrna_mx_mfe_free\(\)](#), [vrna_mx_pf_free\(\)](#)

Parameters

<i>vc</i>	The <code>vrna_fold_compound_t</code> that is to be erased from memory
-----------	------------------------------------------------------------------------

15.53.6.4 `void vrna_fold_compound_add_auxdata (vrna_fold_compound_t * vc, void * data, vrna_callback_free_auxdata * f)`

```
#include <ViennaRNA/data_structures.h>
```

Add auxiliary data to the `vrna_fold_compound_t`.

This function allows one to bind arbitrary data to a `vrna_fold_compound_t` which may later on be used by one of the callback functions, e.g. [vrna_callback_recursion_status\(\)](#). To allow for proper cleanup of the memory occupied by this auxiliary data, the user may also provide a pointer to a cleanup function that free's the corresponding memory. This function will be called automatically when the `vrna_fold_compound_t` is free'd with [vrna_fold_compound_free\(\)](#).

Note

Before attaching the arbitrary data pointer, this function will call the [vrna_callback_free_auxdata\(\)](#) on any pre-existing data that is already attached.

See also

[vrna_callback_free_auxdata\(\)](#)

Parameters

<i>vc</i>	The fold_compound the arbitrary data pointer should be associated with
<i>data</i>	A pointer to an arbitrary data structure
<i>f</i>	A pointer to function that free's memory occupied by the arbitrary data (May be NULL)

15.53.6.5 void vrna_fold_compound_add_callback (vrna_fold_compound_t * vc, vrna_callback_recursion_status * f)

```
#include <ViennaRNA/data_structures.h>
```

Add a recursion status callback to the [vrna_fold_compound_t](#).

Binding a recursion status callback function to a [vrna_fold_compound_t](#) allows one to perform arbitrary operations just before, or after an actual recursive computations, e.g. MFE prediction, is performed by the RNAlib. The callback function will be provided with a pointer to its [vrna_fold_compound_t](#), and a status message. Hence, it has complete access to all variables that influence the recursive computations.

See also

[vrna_callback_recursion_status\(\)](#), [vrna_fold_compound_t](#), [VRNA_STATUS_MFE_PRE](#), [VRNA_STATUS_MFE_POST](#), [VRNA_STATUS_PF_PRE](#), [VRNA_STATUS_PF_POST](#)

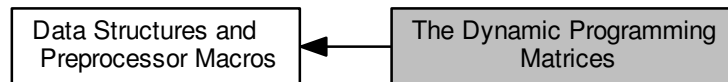
Parameters

<i>vc</i>	The fold_compound the callback function should be attached to
<i>f</i>	The pointer to the recursion status callback function

15.54 The Dynamic Programming Matrices

This module provides interfaces that deal with creation and destruction of dynamic programming matrices used within the RNAlib.

Collaboration diagram for The Dynamic Programming Matrices:



Data Structures

- struct [vrna_mx_mfe_s](#)
Minimum Free Energy (MFE) Dynamic Programming (DP) matrices data structure required within the [vrna_fold_compound_t](#). [More...](#)
- struct [vrna_mx_pf_s](#)
Partition function (PF) Dynamic Programming (DP) matrices data structure required within the [vrna_fold_compound_t](#). [More...](#)

Typedefs

- typedef struct [vrna_mx_mfe_s](#) [vrna_mx_mfe_t](#)
Typename for the Minimum Free Energy (MFE) DP matrices data structure [vrna_mx_mfe_s](#).
- typedef struct [vrna_mx_pf_s](#) [vrna_mx_pf_t](#)
Typename for the Partition Function (PF) DP matrices data structure [vrna_mx_pf_s](#).

Enumerations

Functions

- int [vrna_mx_add](#) ([vrna_fold_compound_t](#) *vc, [vrna_mx_type_e](#) type, unsigned int options)
Add Dynamic Programming (DP) matrices (allocate memory)
- void [vrna_mx_mfe_free](#) ([vrna_fold_compound_t](#) *vc)
Free memory occupied by the Minimum Free Energy (MFE) Dynamic Programming (DP) matrices.
- void [vrna_mx_pf_free](#) ([vrna_fold_compound_t](#) *vc)
Free memory occupied by the Partition Function (PF) Dynamic Programming (DP) matrices.

15.54.1 Detailed Description

This module provides interfaces that deal with creation and destruction of dynamic programming matrices used within the RNAlib.

15.54.2 Data Structure Documentation

15.54.2.1 struct vrna_mx_mfe_s

Minimum Free Energy (MFE) Dynamic Programming (DP) matrices data structure required within the [vrna_fold_compound_t](#).

Data Fields

Common fields for MFE matrices

- [vrna_mx_type_e](#) type
- unsigned int [length](#)
Length of the sequence, therefore an indicator of the size of the DP matrices.

Default DP matrices

Note

These data fields are available if
`vrna_mx_mfe_t.type == VRNA_MX_DEFAULT`

Local Folding DP matrices using window approach

Note

These data fields are available if
`vrna_mx_mfe_t.type == VRNA_MX_WINDOW`

Distance Class DP matrices

Note

These data fields are available if
`vrna_mx_mfe_t.type == VRNA_MX_2DFOLD`

15.54.2.2 struct vrna_mx_pf_s

Partition function (PF) Dynamic Programming (DP) matrices data structure required within the [vrna_fold_compound_t](#).

Data Fields

Common fields for DP matrices

- [vrna_mx_type_e](#) type
- unsigned int [length](#)
- [FLT_OR_DBL](#) * [scale](#)
- [FLT_OR_DBL](#) * [expMLbase](#)

Default PF matrices

Note

These data fields are available if
`vrna_mx_pf_t.type == VRNA_MX_DEFAULT`

Distance Class DP matrices

Note

These data fields are available if
`vrna_mx_pf_t.type == VRNA_MX_2DFOLD`

15.54.3 Enumeration Type Documentation

15.54.3.1 enum vrna_mx_type_e

```
#include <ViennaRNA/dp_matrices.h>
```

An enumerator that is used to specify the type of a polymorphic Dynamic Programming (DP) matrix data structure.

See also

[vrna_mx_mfe_t](#), [vrna_mx_pf_t](#)

Enumerator

VRNA_MX_DEFAULT Default DP matrices.

VRNA_MX_WINDOW DP matrices suitable for local structure prediction using window approach.

See also

[vrna_mfe_window\(\)](#), [vrna_mfe_window_zscore\(\)](#), [pfl_fold\(\)](#)

VRNA_MX_2DFOLD DP matrices suitable for distance class partitioned structure prediction.

See also

[vrna_mfe_TwoD\(\)](#), [vrna_pf_TwoD\(\)](#)

15.54.4 Function Documentation

15.54.4.1 int vrna_mx_add (vrna_fold_compound_t * vc, vrna_mx_type_e type, unsigned int options)

```
#include <ViennaRNA/dp_matrices.h>
```

Add Dynamic Programming (DP) matrices (allocate memory)

This function adds DP matrices of a specific type to the provided [vrna_fold_compound_t](#), such that successive DP recursion can be applied. The function caller has to specify which type of DP matrix is requested, see [vrna_mx_type_e](#), and what kind of recursive algorithm will be applied later on, using the parameters type, and options, respectively. For the latter, Minimum free energy (MFE), and Partition function (PF) computations are distinguished. A third option that may be passed is [VRNA_OPTION_HYBRID](#), indicating that auxiliary DP arrays are required for RNA-RNA interaction prediction.

Note

Usually, there is no need to call this function, since the constructors of [vrna_fold_compound_t](#) are handling all the DP matrix memory allocation.

See also

[vrna_mx_mfe_add\(\)](#), [vrna_mx_pf_add\(\)](#), [vrna_fold_compound\(\)](#), [vrna_fold_compound_comparative\(\)](#), [vrna_fold_compound_free\(\)](#), [vrna_mx_pf_free\(\)](#), [vrna_mx_mfe_free\(\)](#), [vrna_mx_type_e](#), [VRNA_OPTION_MFE](#), [VRNA_OPTION_PF](#), [VRNA_OPTION_HYBRID](#), [VRNA_OPTION_EVAL_ONLY](#)

Parameters

<i>vc</i>	The vrna_fold_compound_t that holds pointers to the DP matrices
<i>type</i>	The type of DP matrices requested
<i>options</i>	Option flags that specify the kind of DP matrices, such as MFE or PF arrays, and auxiliary requirements

Returns

1 if DP matrices were properly allocated and attached, 0 otherwise

15.54.4.2 `void vrna_mx_mfe_free (vrna_fold_compound_t * vc)`

```
#include <ViennaRNA/dp_matrices.h>
```

Free memory occupied by the Minimum Free Energy (MFE) Dynamic Programming (DP) matrices.

See also

[vrna_fold_compound\(\)](#), [vrna_fold_compound_comparative\(\)](#), [vrna_fold_compound_free\(\)](#), [vrna_mx_pf_free\(\)](#)

Parameters

<i>vc</i>	The vrna_fold_compound_t storing the MFE DP matrices that are to be erased from memory
-----------	--------------------------------------------------------------------------------------------------------

15.54.4.3 `void vrna_mx_pf_free (vrna_fold_compound_t * vc)`

```
#include <ViennaRNA/dp_matrices.h>
```

Free memory occupied by the Partition Function (PF) Dynamic Programming (DP) matrices.

See also

[vrna_fold_compound\(\)](#), [vrna_fold_compound_comparative\(\)](#), [vrna_fold_compound_free\(\)](#), [vrna_mx_mfe_free\(\)](#)

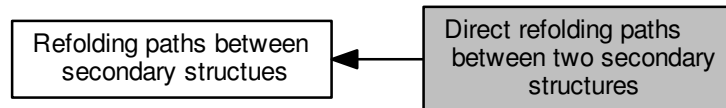
Parameters

<i>vc</i>	The vrna_fold_compound_t storing the PF DP matrices that are to be erased from memory
-----------	-------------------------------------------------------------------------------------------------------

15.55 Direct refolding paths between two secondary structures

Heuristics to explore direct, optimal (re-)folding paths between two secondary structures.

Collaboration diagram for Direct refolding paths between two secondary structures:



Data Structures

- struct [vrna_path_s](#)
An element of a refolding path list. [More...](#)

Typedefs

- typedef struct [vrna_path_s](#) [vrna_path_t](#)
Typename for the refolding path data structure [vrna_path_s](#).
- typedef struct [vrna_path_s](#) [path_t](#)
Old typename of [vrna_path_s](#).

Functions

- int [vrna_path_findpath_saddle](#) ([vrna_fold_compound_t](#) *vc, const char *struc1, const char *struc2, int max)
Find energy of a saddle point between 2 structures (search only direct path)
- [vrna_path_t](#) * [vrna_path_findpath](#) ([vrna_fold_compound_t](#) *vc, const char *s1, const char *s2, int maxkeep)
Find refolding path between 2 structures (search only direct path)
- int [find_saddle](#) (const char *seq, const char *struc1, const char *struc2, int max)
Find energy of a saddle point between 2 structures (search only direct path)
- void [free_path](#) ([vrna_path_t](#) *path)
Free memory allocated by [get_path\(\)](#) function.
- [vrna_path_t](#) * [get_path](#) (const char *seq, const char *s1, const char *s2, int maxkeep)
Find refolding path between 2 structures (search only direct path)

15.55.1 Detailed Description

Heuristics to explore direct, optimal (re-)folding paths between two secondary structures.

15.55.2 Data Structure Documentation

15.55.2.1 struct vrna_path_s

An element of a refolding path list.

See also

[vrna_path_findpath\(\)](#)

Data Fields

- double [en](#)
Free energy of current structure.
- char * [s](#)
Secondary structure in dot-bracket notation.

15.55.3 Typedef Documentation

15.55.3.1 typedef struct vrna_path_s path_t

```
#include <ViennaRNA/findpath.h>
```

Old typename of [vrna_path_s](#).

Deprecated Use [vrna_path_t](#) instead!

15.55.4 Function Documentation

15.55.4.1 int vrna_path_findpath_saddle (vrna_fold_compound_t * vc, const char * struc1, const char * struc2, int max)

```
#include <ViennaRNA/findpath.h>
```

Find energy of a saddle point between 2 structures (search only direct path)

This function uses an implementation of the *findpath* algorithm [5] for near-optimal direct refolding path prediction.

Model details, and energy parameters are used as provided via the parameter 'vc'. The [vrna_fold_compound_t](#) does not require memory for any DP matrices, but requires all most basic init values as one would get from a call like this:

```
vc = vrna_fold_compound(sequence, NULL, VRNA_OPTION_EVAL_ONLY);
```

See also

[vrna_fold_compound\(\)](#), [vrna_fold_compound_t](#), [vrna_path_findpath\(\)](#)

Parameters

<i>vc</i>	The vrna_fold_compound_t with precomputed sequence encoding and model details
<i>struc1</i>	The start structure in dot-bracket notation
<i>struc2</i>	The target structure in dot-bracket notation
<i>max</i>	A number specifying how many structures are being kept at each step during the search

Returns

The saddle energy in 10cal/mol

15.55.4.2 `vrna_path_t* vrna_path_findpath (vrna_fold_compound_t * vc, const char * s1, const char * s2, int maxkeep)`

```
#include <ViennaRNA/findpath.h>
```

Find refolding path between 2 structures (search only direct path)

This function uses an implementation of the *findpath* algorithm [5] for near-optimal direct refolding path prediction.

Model details, and energy parameters are used as provided via the parameter 'vc'. The [vrna_fold_compound_t](#) does not require memory for any DP matrices, but requires all most basic init values as one would get from a call like this:

```
vc = vrna_fold_compound(sequence, NULL, VRNA_OPTION_EVAL_ONLY);
```

See also

[vrna_fold_compound\(\)](#), [vrna_fold_compound_t](#), [vrna_path_findpath_saddle\(\)](#)

Parameters

<i>vc</i>	The vrna_fold_compound_t with precomputed sequence encoding and model details
<i>s1</i>	The start structure in dot-bracket notation
<i>s2</i>	The target structure in dot-bracket notation
<i>maxkeep</i>	A number specifying how many structures are being kept at each step during the search

Returns

The saddle energy in 10cal/mol

15.55.4.3 `int find_saddle (const char * seq, const char * struc1, const char * struc2, int max)`

```
#include <ViennaRNA/findpath.h>
```

Find energy of a saddle point between 2 structures (search only direct path)

Parameters

<i>seq</i>	RNA sequence
<i>struc1</i>	A pointer to the character array where the first secondary structure in dot-bracket notation will be written to
<i>struc2</i>	A pointer to the character array where the second secondary structure in dot-bracket notation will be written to
<i>max</i>	integer how many strutures are being kept during the search

Returns

the saddle energy in 10cal/mol

15.55.4.4 `void free_path (vrna_path_t * path)`

`#include <ViennaRNA/findpath.h>`

Free memory allocated by `get_path()` function.

Parameters

<i>path</i>	pointer to memory to be freed
-------------	-------------------------------

15.55.4.5 `vrna_path_t* get_path (const char * seq, const char * s1, const char * s2, int maxkeep)`

`#include <ViennaRNA/findpath.h>`

Find refolding path between 2 structures (search only direct path)

Parameters

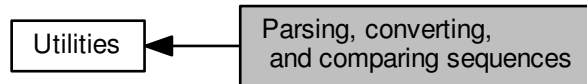
<i>seq</i>	RNA sequence
<i>s1</i>	A pointer to the character array where the first secondary structure in dot-bracket notation will be written to
<i>s2</i>	A pointer to the character array where the second secondary structure in dot-bracket notation will be written to
<i>maxkeep</i>	integer how many strutures are being kept during the search

Returns

direct refolding path between two structures

15.56 Parsing, converting, and comparing sequences

Collaboration diagram for Parsing, converting, and comparing sequences:



- `#define XSTR(s) STR(s)`
Stringify a macro after expansion.
- `#define STR(s) #s`
Stringify a macro argument.
- `#define FILENAME_MAX_LENGTH 80`
Maximum length of filenames that are generated by our programs.
- `#define FILENAME_ID_LENGTH 42`
Maximum length of id taken from fasta header for filename generation.
- `char * vrna_strdup_printf (const char *format,...)`
Safely create a formatted string.
- `char * vrna_strdup_vprintf (const char *format, va_list argp)`
Safely create a formatted string.
- `int vrna_strcat_printf (char **dest, const char *format,...)`
Safely append a formatted string to another string.
- `int vrna_strcat_vprintf (char **dest, const char *format, va_list args)`
Safely append a formatted string to another string.
- `char * vrna_random_string (int l, const char symbols[])`
Create a random string using characters from a specified symbol set.
- `int vrna_hamming_distance (const char *s1, const char *s2)`
Calculate hamming distance between two sequences.
- `int vrna_hamming_distance_bound (const char *s1, const char *s2, int n)`
Calculate hamming distance between two sequences up to a specified length.
- `void vrna_seq_toRNA (char *sequence)`
Convert an input sequence (possibly containing DNA alphabet characters) to RNA alphabet.
- `void vrna_seq_toupper (char *sequence)`
Convert an input sequence to uppercase.
- `char * vrna_cut_point_insert (const char *string, int cp)`
Add a separating '&' character into a string according to cut-point position.
- `char * vrna_cut_point_remove (const char *string, int *cp)`
Remove a separating '&' character from a string.

15.56.1 Detailed Description

15.56.2 Macro Definition Documentation

15.56.2.1 `#define FILENAME_MAX_LENGTH 80`

```
#include <ViennaRNA/string_utils.h>
```

Maximum length of filenames that are generated by our programs.

This definition should be used throughout the complete ViennaRNA package wherever a static array holding file-names of output files is declared.

15.56.2.2 `#define FILENAME_ID_LENGTH 42`

```
#include <ViennaRNA/string_utils.h>
```

Maximum length of id taken from fasta header for filename generation.

this has to be smaller than `FILENAME_MAX_LENGTH` since in most cases, some suffix will be appended to the ID

15.56.3 Function Documentation

15.56.3.1 `char* vrna_strdup_printf (const char * format, ...)`

```
#include <ViennaRNA/string_utils.h>
```

Safely create a formatted string.

This function is a safe implementation for creating a formatted character array, similar to *sprintf*. Internally, it uses the *asprintf* function if available to dynamically allocate a large enough character array to store the supplied content. If *asprintf* is not available, mimic it's behavior using *vsnprintf*.

Note

The returned pointer of this function should always be passed to *free()* to release the allocated memory

See also

[vrna_strdup_vprintf\(\)](#), [vrna_strcat_printf\(\)](#)

Parameters

<i>format</i>	The format string (See also <i>asprintf</i>)
...	The list of variables used to fill the format string

Returns

The formatted, null-terminated string, or NULL if something has gone wrong

15.56.3.2 `char* vrna_strdup_vprintf (const char * format, va_list argp)`

```
#include <ViennaRNA/string_utils.h>
```

Safely create a formatted string.

This function is the *va_list* version of [vrna_strdup_printf\(\)](#)

Note

The returned pointer of this function should always be passed to *free()* to release the allocated memory

See also

[vrna_strdup_printf\(\)](#), [vrna_strcat_printf\(\)](#), [vrna_strcat_vprintf\(\)](#)

Parameters

<i>format</i>	The format string (See also asprintf)
...	The list of variables used to fill the format string

Returns

The formatted, null-terminated string, or NULL if something has gone wrong

15.56.3.3 `int vrna_strcat_printf (char ** dest, const char * format, ...)`

```
#include <ViennaRNA/string_utils.h>
```

Safely append a formatted string to another string.

This function is a safe implementation for appending a formatted character array, similar to a combination of *strcat* and *sprintf*. The function automatically allocates enough memory to store both, the previous content stored at *dest* and the appended format string. If the *dest* pointer is NULL, the function allocate memory only for the format string. The function returns the number of characters in the resulting string or -1 in case of an error.

See also

[vrna_strcat_vprintf\(\)](#), [vrna_strdup_printf\(\)](#), [vrna_strdup_vprintf\(\)](#)

Parameters

<i>dest</i>	The address of a char *pointer where the formatted string is to be appended
<i>format</i>	The format string (See also sprintf)
...	The list of variables used to fill the format string

Returns

The number of characters in the final string, or -1 on error

15.56.3.4 `int vrna_strcat_vprintf (char ** dest, const char * format, va_list args)`

```
#include <ViennaRNA/string_utils.h>
```

Safely append a formatted string to another string.

This function is the *va_list* version of [vrna_strcat_printf\(\)](#)

See also

[vrna_strcat_printf\(\)](#), [vrna_strdup_printf\(\)](#), [vrna_strdup_vprintf\(\)](#)

Parameters

<i>dest</i>	The address of a char *pointer where the formatted string is to be appended
<i>format</i>	The format string (See also <code>printf</code>)
...	The list of variables used to fill the format string

Returns

The number of characters in the final string, or -1 on error

15.56.3.5 `char* vrna_random_string (int l, const char symbols[])`

```
#include <ViennaRNA/string_utils.h>
```

Create a random string using characters from a specified symbol set.

Parameters

<i>l</i>	The length of the sequence
<i>symbols</i>	The symbol set

Returns

A random string of length 'l' containing characters from the symbolset

15.56.3.6 `int vrna_hamming_distance (const char * s1, const char * s2)`

```
#include <ViennaRNA/string_utils.h>
```

Calculate hamming distance between two sequences.

Parameters

<i>s1</i>	The first sequence
<i>s2</i>	The second sequence

Returns

The hamming distance between *s1* and *s2*

15.56.3.7 `int vrna_hamming_distance_bound (const char * s1, const char * s2, int n)`

```
#include <ViennaRNA/string_utils.h>
```

Calculate hamming distance between two sequences up to a specified length.

This function is similar to `vrna_hamming_distance()` but instead of comparing both sequences up to their actual length only the first '*n*' characters are taken into account

Parameters

<i>s1</i>	The first sequence
<i>s2</i>	The second sequence
<i>n</i>	The length of the subsequences to consider (starting from the 5' end)

Returns

The hamming distance between *s1* and *s2*

15.56.3.8 `void vrna_seq_toRNA (char * sequence)`

```
#include <ViennaRNA/string_utils.h>
```

Convert an input sequence (possibly containing DNA alphabet characters) to RNA alphabet.

This function substitutes *T* and *t* with *U* and *u*, respectively

Parameters

<i>sequence</i>	The sequence to be converted
-----------------	------------------------------

15.56.3.9 `void vrna_seq_toupper (char * sequence)`

```
#include <ViennaRNA/string_utils.h>
```

Convert an input sequence to uppercase.

Parameters

<i>sequence</i>	The sequence to be converted
-----------------	------------------------------

15.56.3.10 `char* vrna_cut_point_insert (const char * string, int cp)`

```
#include <ViennaRNA/string_utils.h>
```

Add a separating '&' character into a string according to cut-point position.

If the cut-point position is less or equal to zero, this function just returns a copy of the provided string. Otherwise, the cut-point character is set at the corresponding position

Parameters

<i>string</i>	The original string
<i>cp</i>	The cut-point position

Returns

A copy of the provided string including the cut-point character

15.56.3.11 `char* vrna_cut_point_remove (const char * string, int * cp)`

```
#include <ViennaRNA/string_utils.h>
```

Remove a separating '&' character from a string.

This function removes the cut-point indicating '&' character from a string and memorizes its position in a provided integer variable. If not '&' is found in the input, the integer variable is set to -1. The function returns a copy of the input string with the '&' being sliced out.

Parameters

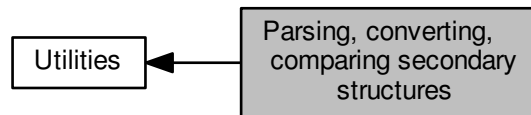
<i>string</i>	The original string
<i>cp</i>	The cut-point position

Returns

A copy of the input string with the '&' being sliced out

15.57 Parsing, converting, comparing secondary structures

Collaboration diagram for Parsing, converting, comparing secondary structures:



Files

- file [RNAstruct.h](#)
Parsing and Coarse Graining of Structures.

Functions

- char * [b2HIT](#) (const char *structure)
Converts the full structure from bracket notation to the HIT notation including root.
- char * [b2C](#) (const char *structure)
Converts the full structure from bracket notation to the a coarse grained notation using the 'H' 'B' 'I' 'M' and 'R' identifiers.
- char * [b2Shapiro](#) (const char *structure)
Converts the full structure from bracket notation to the weighted coarse grained notation using the 'H' 'B' 'I' 'M' 'S' 'E' and 'R' identifiers.
- char * [add_root](#) (const char *structure)
Adds a root to an un-rooted tree in any except bracket notation.
- char * [expand_Shapiro](#) (const char *coarse)
Inserts missing 'S' identifiers in unweighted coarse grained structures as obtained from [b2C\(\)](#).
- char * [expand_Full](#) (const char *structure)
Convert the full structure from bracket notation to the expanded notation including root.
- char * [unexpand_Full](#) (const char *ffull)
Restores the bracket notation from an expanded full or HIT tree, that is any tree using only identifiers 'U' 'P' and 'R'.
- char * [unweight](#) (const char *wcoarse)
Strip weights from any weighted tree.
- void [unexpand_aligned_F](#) (char *align[2])
Converts two aligned structures in expanded notation.
- void [parse_structure](#) (const char *structure)
Collects a statistic of structure elements of the full structure in bracket notation.

Variables

- int `loop_size` [STRUC]
contains a list of all loop sizes. loop_size[0] contains the number of external bases.
- int `helix_size` [STRUC]
contains a list of all stack sizes.
- int `loop_degree` [STRUC]
contains the corresponding list of loop degrees.
- int `loops`
contains the number of loops (and therefore of stacks).
- int `unpaired`
contains the number of unpaired bases.
- int `pairs`
contains the number of base pairs in the last parsed structure.

- typedef struct `vrna_hx_s` `vrna_hx_t`
Convenience typedef for data structure `vrna_hx_s`.
- char * `vrna_db_pack` (const char *struc)
Pack secondary structure, 5:1 compression using base 3 encoding.
- char * `vrna_db_unpack` (const char *packed)
Unpack secondary structure previously packed with `vrna_db_pack()`
- short * `vrna_ptable` (const char *structure)
Create a pair table of a secondary structure.
- short * `vrna_pt_pk_get` (const char *structure)
Create a pair table of a secondary structure (pseudo-knot version)
- short * `vrna_ptable_copy` (const short *pt)
Get an exact copy of a pair table.
- short * `vrna_pt_ali_get` (const char *structure)
Create a pair table of a secondary structure (snoop align version)
- short * `vrna_pt_snoop_get` (const char *structure)
Create a pair table of a secondary structure (snoop version)
- int * `vrna_loopidx_from_ptable` (const short *pt)
Get a loop index representation of a structure.
- char * `vrna_db_from_ptable` (short *pt)
Convert a pair table into dot-parenthesis notation.
- int `vrna_bp_distance` (const char *str1, const char *str2)
Compute the "base pair" distance between two secondary structures s1 and s2.
- unsigned int * `vrna_refBPcnt_matrix` (const short *reference_pt, unsigned int turn)
Make a reference base pair count matrix.
- unsigned int * `vrna_refBPdist_matrix` (const short *pt1, const short *pt2, unsigned int turn)
Make a reference base pair distance matrix.
- char * `vrna_db_from_probs` (const FLT_OR_DBL *pr, unsigned int length)
Create a dot-bracket like structure string from base pair probability matrix.
- char * `vrna_bpp_symbol` (const float *x)
Get a pseudo dot bracket notation for a given probability information.
- char * `vrna_db_from_bp_stack` (`vrna_bp_stack_t` *bp, unsigned int length)
Create a dot-bracket/parenthesis structure from backtracking stack.
- `vrna_plist_t` * `vrna_plist` (const char *struc, float pr)
Create a `vrna_plist_t` from a dot-bracket string.
- `vrna_plist_t` * `vrna_plist_from_probs` (`vrna_fold_compound_t` *vc, double cut_off)

- Create a `vrna_plist_t` from base pair probability matrix.*
- char * `vrna_db_from_plist` (`vrna_plist_t` *pairs, unsigned int n)
- Convert a list of base pairs into dot-bracket notation.*
- void `assign_plist_from_db` (`vrna_plist_t` **pl, const char *struc, float pr)
- Create a `vrna_plist_t` from a dot-bracket string.*
- char * `pack_structure` (const char *struc)
- Pack secondary secondary structure, 5:1 compression using base 3 encoding.*
- char * `unpack_structure` (const char *packed)
- Unpack secondary structure previously packed with `pack_structure()`*
- short * `make_pair_table` (const char *structure)
- Create a pair table of a secondary structure.*
- short * `copy_pair_table` (const short *pt)
- Get an exact copy of a pair table.*
- short * `alimake_pair_table` (const char *structure)
- short * `make_pair_table_snoop` (const char *structure)
- int `bp_distance` (const char *str1, const char *str2)
- Compute the "base pair" distance between two secondary structures s1 and s2.*
- unsigned int * `make_referenceBP_array` (short *reference_pt, unsigned int turn)
- Make a reference base pair count matrix.*
- unsigned int * `compute_BPdifferences` (short *pt1, short *pt2, unsigned int turn)
- Make a reference base pair distance matrix.*
- void `assign_plist_from_pr` (`vrna_plist_t` **pl, `FLT_OR_DBL` *probs, int length, double cutoff)
- Create a `vrna_plist_t` from a probability matrix.*
- void `parenthesis_structure` (char *structure, `vrna_bp_stack_t` *bp, int length)
- Create a dot-bracket/parenthesis structure from backtracking stack.*
- void `parenthesis_zuker` (char *structure, `vrna_bp_stack_t` *bp, int length)
- Create a dot-bracket/parenthesis structure from backtracking stack obtained by Zuker suboptimal calculation in `cofold.c`.*
- void `bppm_to_structure` (char *structure, `FLT_OR_DBL` *pr, unsigned int length)
- Create a dot-bracket like structure string from base pair probability matrix.*
- char `bppm_symbol` (const float *x)
- Get a pseudo dot bracket notation for a given probability information.*

15.57.1 Detailed Description

15.57.2 Function Documentation

15.57.2.1 char* b2HIT (const char * structure)

```
#include <ViennaRNA/RNAstruct.h>
```

Converts the full structure from bracket notation to the HIT notation including root.

Parameters

<code>structure</code>	
------------------------	--

Returns**15.57.2.2** `char* b2C (const char * structure)`

```
#include <ViennaRNA/RNAstruct.h>
```

Converts the full structure from bracket notation to the a coarse grained notation using the 'H' 'B' 'I' 'M' and 'R' identifiers.

Parameters

<i>structure</i>	
------------------	--

Returns**15.57.2.3** `char* b2Shapiro (const char * structure)`

```
#include <ViennaRNA/RNAstruct.h>
```

Converts the full structure from bracket notation to the *weighted* coarse grained notation using the 'H' 'B' 'I' 'M' 'S' 'E' and 'R' identifiers.

Parameters

<i>structure</i>	
------------------	--

Returns**15.57.2.4** `char* add_root (const char * structure)`

```
#include <ViennaRNA/RNAstruct.h>
```

Adds a root to an un-rooted tree in any except bracket notation.

Parameters

<i>structure</i>	
------------------	--

Returns

15.57.2.5 char* expand_Shapiro (const char * *coarse*)

```
#include <ViennaRNA/RNAstruct.h>
```

Inserts missing 'S' identifiers in unweighted coarse grained structures as obtained from [b2C\(\)](#).

Parameters

<i>coarse</i>	
---------------	--

Returns**15.57.2.6** char* expand_Full (const char * *structure*)

```
#include <ViennaRNA/RNAstruct.h>
```

Convert the full structure from bracket notation to the expanded notation including root.

Parameters

<i>structure</i>	
------------------	--

Returns**15.57.2.7** char* unexpand_Full (const char * *ffull*)

```
#include <ViennaRNA/RNAstruct.h>
```

Restores the bracket notation from an expanded full or HIT tree, that is any tree using only identifiers 'U' 'P' and 'R'.

Parameters

<i>ffull</i>	
--------------	--

Returns**15.57.2.8** char* unweight (const char * *wcoarse*)

```
#include <ViennaRNA/RNAstruct.h>
```

Strip weights from any weighted tree.

Parameters

<i>wcoarse</i>	
----------------	--

Returns

15.57.2.9 void unexpand_aligned_F (char * *align*[2])

```
#include <ViennaRNA/RNAstruct.h>
```

Converts two aligned structures in expanded notation.

Takes two aligned structures as produced by [tree_edit_distance\(\)](#) function back to bracket notation with '_' as the gap character. The result overwrites the input.

Parameters

<i>align</i>	
--------------	--

15.57.2.10 void parse_structure (const char * *structure*)

```
#include <ViennaRNA/RNAstruct.h>
```

Collects a statistic of structure elements of the full structure in bracket notation.

The function writes to the following global variables: [loop_size](#), [loop_degree](#), [helix_size](#), [loops](#), [pairs](#), [unpaired](#)

Parameters

<i>structure</i>	
------------------	--

Returns

15.57.2.11 char* vrna_db_pack (const char * *struc*)

```
#include <ViennaRNA/structure_utils.h>
```

Pack secondary secondary structure, 5:1 compression using base 3 encoding.

Returns a binary string encoding of the secondary structure using a 5:1 compression scheme. The string is NULL terminated and can therefore be used with standard string functions such as strcmp(). Useful for programs that need to keep many structures in memory.

See also

[vrna_db_unpack\(\)](#)

Parameters

<i>struct</i>	The secondary structure in dot-bracket notation
---------------	-------------------------------------------------

Returns

The binary encoded structure

15.57.2.12 `char* vrna_db_unpack (const char * packed)`

```
#include <ViennaRNA/structure_utils.h>
```

Unpack secondary structure previously packed with `vrna_db_pack()`

Translate a compressed binary string produced by `vrna_db_pack()` back into the familiar dot-bracket notation.

See also

[vrna_db_pack\(\)](#)

Parameters

<i>packed</i>	The binary encoded packed secondary structure
---------------	-----------------------------------------------

Returns

The unpacked secondary structure in dot-bracket notation

15.57.2.13 `short* vrna_ptable (const char * structure)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a pair table of a secondary structure.

Returns a newly allocated table, such that `table[i]=j` if (i,j) pair or 0 if i is unpaired, `table[0]` contains the length of the structure.

Parameters

<i>structure</i>	The secondary structure in dot-bracket notation
------------------	-------------------------------------------------

Returns

A pointer to the created `pair_table`

15.57.2.14 `short* vrna_pt_pk_get (const char * structure)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a pair table of a secondary structure (pseudo-knot version)

Returns a newly allocated table, such that table[i]=j if (i,j) pair or 0 if i is unpaired, table[0] contains the length of the structure.

In contrast to [vrna_ptable\(\)](#) this function also recognizes the base pairs denoted by '[' and ']' brackets.

Parameters

<i>structure</i>	The secondary structure in (extended) dot-bracket notation
------------------	------------------------------------------------------------

Returns

A pointer to the created pair_table

15.57.2.15 `short* vrna_ptable_copy (const short * pt)`

```
#include <ViennaRNA/structure_utils.h>
```

Get an exact copy of a pair table.

Parameters

<i>pt</i>	The pair table to be copied
-----------	-----------------------------

Returns

A pointer to the copy of 'pt'

15.57.2.16 `short* vrna_pt_snoop_get (const char * structure)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a pair table of a secondary structure (snoop version)

returns a newly allocated table, such that: table[i]=j if (i,j) pair or 0 if i is unpaired, table[0] contains the length of the structure. The special pseudoknotted H/ACA-mRNA structure is taken into account.

15.57.2.17 `char* vrna_db_from_ptable (short * pt)`

```
#include <ViennaRNA/structure_utils.h>
```

Convert a pair table into dot-parenthesis notation.

Parameters

<i>pt</i>	The pair table to be copied
-----------	-----------------------------

Returns

A char pointer to the dot-bracket string

15.57.2.18 `int vrna_bp_distance (const char * str1, const char * str2)`

```
#include <ViennaRNA/structure_utils.h>
```

Compute the "base pair" distance between two secondary structures *s1* and *s2*.

The sequences should have the same length. dist = number of base pairs in one structure but not in the other same as edit distance with open-pair close-pair as move-set

Parameters

<i>str1</i>	First structure in dot-bracket notation
<i>str2</i>	Second structure in dot-bracket notation

Returns

The base pair distance between *str1* and *str2*

15.57.2.19 `unsigned int* vrna_refBPcnt_matrix (const short * reference_pt, unsigned int turn)`

```
#include <ViennaRNA/structure_utils.h>
```

Make a reference base pair count matrix.

Get an upper triangular matrix containing the number of basepairs of a reference structure for each interval [i,j] with i<j. Access it via *iindx*!!!

15.57.2.20 `unsigned int* vrna_refBPdist_matrix (const short * pt1, const short * pt2, unsigned int turn)`

```
#include <ViennaRNA/structure_utils.h>
```

Make a reference base pair distance matrix.

Get an upper triangular matrix containing the base pair distance of two reference structures for each interval [i,j] with i<j. Access it via *iindx*!!!

15.57.2.21 `char* vrna_db_from_bp_stack (vrna_bp_stack_t * bp, unsigned int length)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a dot-bracket/parenthesis structure from backtracking stack.

This function is capable to create dot-bracket structures from suboptimal structure prediction sensu M. Zuker

Parameters

<i>bp</i>	Base pair stack containing the traced base pairs
<i>length</i>	The length of the structure

Returns

The secondary structure in dot-bracket notation as provided in the input

15.57.2.22 `vrna_plist_t* vrna_plist (const char * struc, float pr)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a [vrna_plist_t](#) from a dot-bracket string.

The dot-bracket string is parsed and for each base pair an entry in the plist is created. The probability of each pair in the list is set by a function parameter.

The end of the plist is marked by sequence positions *i* as well as *j* equal to 0. This condition should be used to stop looping over its entries

Parameters

<i>struc</i>	The secondary structure in dot-bracket notation
<i>pr</i>	The probability for each base pair used in the plist

Returns

The plist array

15.57.2.23 `vrna_plist_t* vrna_plist_from_probs (vrna_fold_compound_t * vc, double cut_off)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a [vrna_plist_t](#) from base pair probability matrix.

The probability matrix provided via the [vrna_fold_compound_t](#) is parsed and all pair probabilities above the given threshold are used to create an entry in the plist

The end of the plist is marked by sequence positions *i* as well as *j* equal to 0. This condition should be used to stop looping over its entries

Parameters

<i>in</i>	<i>vc</i>	The fold compound
<i>in</i>	<i>cut_off</i>	The cutoff value

Returns

A pointer to the plist that is to be created

15.57.2.24 `char* vrna_db_from_plist (vrna_plist_t * pairs, unsigned int n)`

```
#include <ViennaRNA/structure_utils.h>
```

Convert a list of base pairs into dot-bracket notation.

See also

[vrna_plist\(\)](#)

Parameters

<i>pairs</i>	A vrna_plist_t containing the pairs to be included in the dot-bracket string
<i>n</i>	The length of the structure (number of nucleotides)

Returns

The dot-bracket string containing the provided base pairs

15.57.2.25 `void assign_plist_from_db (vrna_plist_t ** pl, const char * struc, float pr)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a [vrna_plist_t](#) from a dot-bracket string.

The dot-bracket string is parsed and for each base pair an entry in the plist is created. The probability of each pair in the list is set by a function parameter.

The end of the plist is marked by sequence positions *i* as well as *j* equal to 0. This condition should be used to stop looping over its entries

Deprecated Use [vrna_plist\(\)](#) instead

Parameters

<i>pl</i>	A pointer to the vrna_plist_t that is to be created
<i>struc</i>	The secondary structure in dot-bracket notation
<i>pr</i>	The probability for each base pair

15.57.2.26 `char* pack_structure (const char * struc)`

```
#include <ViennaRNA/structure_utils.h>
```

Pack secondary structure, 5:1 compression using base 3 encoding.

Returns a binary string encoding of the secondary structure using a 5:1 compression scheme. The string is NULL terminated and can therefore be used with standard string functions such as `strcmp()`. Useful for programs that need to keep many structures in memory.

Deprecated Use `vrna_db_pack()` as a replacement

Parameters

<i>struc</i>	The secondary structure in dot-bracket notation
--------------	-------------------------------------------------

Returns

The binary encoded structure

15.57.2.27 `char* unpack_structure (const char * packed)`

```
#include <ViennaRNA/structure_utils.h>
```

Unpack secondary structure previously packed with `pack_structure()`

Translate a compressed binary string produced by `pack_structure()` back into the familiar dot-bracket notation.

Deprecated Use `vrna_db_unpack()` as a replacement

Parameters

<i>packed</i>	The binary encoded packed secondary structure
---------------	-----------------------------------------------

Returns

The unpacked secondary structure in dot-bracket notation

15.57.2.28 `short* make_pair_table (const char * structure)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a pair table of a secondary structure.

Returns a newly allocated table, such that `table[i]=j` if (i,j) pair or 0 if i is unpaired, `table[0]` contains the length of the structure.

Deprecated Use `vrna_ptable()` instead

Parameters

<i>structure</i>	The secondary structure in dot-bracket notation
------------------	-------------------------------------------------

Returns

A pointer to the created pair_table

15.57.2.29 `short* copy_pair_table (const short * pt)`

```
#include <ViennaRNA/structure_utils.h>
```

Get an exact copy of a pair table.

Deprecated Use `vrna_ptable_copy()` instead

Parameters

<i>pt</i>	The pair table to be copied
-----------	-----------------------------

Returns

A pointer to the copy of 'pt'

15.57.2.30 `short* alimake_pair_table (const char * structure)`

```
#include <ViennaRNA/structure_utils.h>
```

Pair table for snoop align

Deprecated Use `vrna_pt_ali_get()` instead!

15.57.2.31 `short* make_pair_table_snoop (const char * structure)`

```
#include <ViennaRNA/structure_utils.h>
```

returns a newly allocated table, such that: table[i]=j if (i,j) pair or 0 if i is unpaired, table[0] contains the length of the structure. The special pseudoknotted H/ACA-mRNA structure is taken into account.

Deprecated Use `vrna_pt_snoop_get()` instead!

15.57.2.32 `int bp_distance (const char * str1, const char * str2)`

```
#include <ViennaRNA/structure_utils.h>
```

Compute the "base pair" distance between two secondary structures s1 and s2.

The sequences should have the same length. dist = number of base pairs in one structure but not in the other same as edit distance with open-pair close-pair as move-set

Deprecated Use `vrna_bp_distance` instead

Parameters

<i>str1</i>	First structure in dot-bracket notation
<i>str2</i>	Second structure in dot-bracket notation

Returns

The base pair distance between *str1* and *str2*

15.57.2.33 `unsigned int* make_referenceBP_array (short * reference_pt, unsigned int turn)`

```
#include <ViennaRNA/structure_utils.h>
```

Make a reference base pair count matrix.

Get an upper triangular matrix containing the number of basepairs of a reference structure for each interval $[i,j]$ with $i < j$. Access it via `iindx!!!`

Deprecated Use `vrna_refBPcnt_matrix()` instead

15.57.2.34 `unsigned int* compute_BPdifferences (short * pt1, short * pt2, unsigned int turn)`

```
#include <ViennaRNA/structure_utils.h>
```

Make a reference base pair distance matrix.

Get an upper triangular matrix containing the base pair distance of two reference structures for each interval $[i,j]$ with $i < j$. Access it via `iindx!!!`

Deprecated Use `vrna_refBPdist_matrix()` instead

15.57.2.35 `void assign_plist_from_pr (vrna_plist_t ** pl, FLT_OR_DBL * probs, int length, double cutoff)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a `vrna_plist_t` from a probability matrix.

The probability matrix given is parsed and all pair probabilities above the given threshold are used to create an entry in the plist

The end of the plist is marked by sequence positions i as well as j equal to 0. This condition should be used to stop looping over its entries

Note

This function is threadsafe

Deprecated Use `vrna_plist_from_probs()` instead!

Parameters

out	<i>pl</i>	A pointer to the <code>vrna_plist_t</code> that is to be created
in	<i>probs</i>	The probability matrix used for creating the plist
in	<i>length</i>	The length of the RNA sequence
in	<i>cutoff</i>	The cutoff value

15.57.2.36 `void parenthesis_structure (char * structure, vrna_bp_stack_t * bp, int length)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a dot-bracket/parenthesis structure from backtracking stack.

Deprecated use `vrna_parenthesis_structure()` instead

Note

This function is threadsafe

15.57.2.37 `void parenthesis_zuker (char * structure, vrna_bp_stack_t * bp, int length)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a dot-bracket/parenthesis structure from backtracking stack obtained by zuker suboptimal calculation in `cofold.c`.

Deprecated use `vrna_parenthesis_zuker` instead

Note

This function is threadsafe

15.57.2.38 `void bppm_to_structure (char * structure, FLT_OR_DBL * pr, unsigned int length)`

```
#include <ViennaRNA/structure_utils.h>
```

Create a dot-bracket like structure string from base pair probability matrix.

Deprecated Use `vrna_db_from_probs()` instead!

15.57.2.39 `char bppm_symbol (const float * x)`

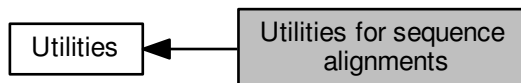
```
#include <ViennaRNA/structure_utils.h>
```

Get a pseudo dot bracket notation for a given probability information.

Deprecated Use `vrna_bpp_symbol()` instead!

15.58 Utilities for sequence alignments

Collaboration diagram for Utilities for sequence alignments:



- typedef struct [vrna_pinfo_s](#) vrna_pinfo_t

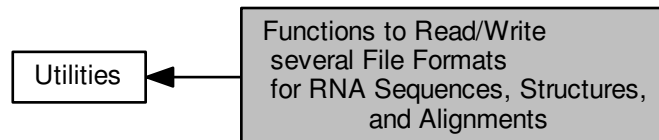
Typename for the base pair info representing data structure [vrna_pinfo_s](#).

15.58.1 Detailed Description

15.59 Functions to Read/Write several File Formats for RNA Sequences, Structures, and Alignments

Functions dealing with file formats for RNA sequences, structures, and alignments.

Collaboration diagram for Functions to Read/Write several File Formats for RNA Sequences, Structures, and Alignments:



Files

- file [commands.h](#)
Parse and apply different commands that alter the behavior of secondary structure prediction and evaluation.
- file [file_formats.h](#)
Read and write different file formats for RNA sequences, structures.
- file [file_formats_msa.h](#)
Functions dealing with file formats for Multiple Sequence Alignments (MSA)
- file [file_utils.h](#)
Several utilities for file handling.
- file [ribo.h](#)
Parse RiboSum Scoring Matrices for Covariance Scoring of Alignments.

Macros

- `#define VRNA_FILE_FORMAT_MSA_CLUSTAL 1U`
Option flag indicating ClustalW formatted files.
- `#define VRNA_FILE_FORMAT_MSA_STOCKHOLM 2U`
Option flag indicating Stockholm 1.0 formatted files.
- `#define VRNA_FILE_FORMAT_MSA_FASTA 4U`
Option flag indicating FASTA (Pearson) formatted files.
- `#define VRNA_FILE_FORMAT_MSA_MAF 8U`
Option flag indicating MAF formatted files.
- `#define VRNA_FILE_FORMAT_MSA_DEFAULT`
Option flag indicating the set of default file formats.
- `#define VRNA_FILE_FORMAT_MSA_NOCHECK 4096U`
Option flag to disable validation of the alignment.
- `#define VRNA_FILE_FORMAT_MSA_UNKNOWN 8192U`
Return flag of [vrna_file_msa_detect_format\(\)](#) to indicate unknown or malformed alignment.

Functions

- int [vrna_file_msa_read](#) (const char *filename, char ***names, char ***aln, char **id, char **structure, unsigned int options)
Read a multiple sequence alignment from file.
- int [vrna_file_msa_read_record](#) (FILE *fp, char ***names, char ***aln, char **id, char **structure, unsigned int options)
Read a multiple sequence alignment from file handle.
- unsigned int [vrna_file_msa_detect_format](#) (const char *filename, unsigned int options)
Detect the format of a multiple sequence alignment file.
- void [vrna_file_copy](#) (FILE *from, FILE *to)
Inefficient 'cp'.
- char * [vrna_read_line](#) (FILE *fp)
Read a line of arbitrary length from a stream.
- int [vrna_mkdir_p](#) (const char *path)
Recursively create a directory tree.
- char * [vrna_basename](#) (const char *path)
Extract the filename from a file path.
- char * [vrna_dirname](#) (const char *path)
Extract the directory part of a file path.

- typedef struct [vrna_command_s](#) [vrna_cmd_t](#)
Typename for the command representing data structure [vrna_command_s](#).

- void [vrna_file_helixlist](#) (const char *seq, const char *db, float energy, FILE *file)
Print a secondary structure as helix list.

15.59.1 Detailed Description

Functions dealing with file formats for RNA sequences, structures, and alignments.

15.59.2 Macro Definition Documentation

15.59.2.1 #define VRNA_FILE_FORMAT_MSA_CLUSTAL 1U

```
#include <ViennaRNA/file_formats_msa.h>
```

Option flag indicating ClustalW formatted files.

See also

[vrna_file_msa_read\(\)](#), [vrna_file_msa_read_record\(\)](#), [vrna_file_msa_detect_format\(\)](#)

15.59.2.2 #define VRNA_FILE_FORMAT_MSA_STOCKHOLM 2U

```
#include <ViennaRNA/file_formats_msa.h>
```

Option flag indicating Stockholm 1.0 formatted files.

See also

[vrna_file_msa_read\(\)](#), [vrna_file_msa_read_record\(\)](#), [vrna_file_msa_detect_format\(\)](#)

15.59.2.3 #define VRNA_FILE_FORMAT_MSA_FASTA 4U

```
#include <ViennaRNA/file_formats_msa.h>
```

Option flag indicating FASTA (Pearson) formatted files.

See also

[vrna_file_msa_read\(\)](#), [vrna_file_msa_read_record\(\)](#), [vrna_file_msa_detect_format\(\)](#)

15.59.2.4 #define VRNA_FILE_FORMAT_MSA_MAF 8U

```
#include <ViennaRNA/file_formats_msa.h>
```

Option flag indicating MAF formatted files.

See also

[vrna_file_msa_read\(\)](#), [vrna_file_msa_read_record\(\)](#), [vrna_file_msa_detect_format\(\)](#)

15.59.2.5 #define VRNA_FILE_FORMAT_MSA_DEFAULT

```
#include <ViennaRNA/file_formats_msa.h>
```

Value:

```
( \
    VRNA_FILE_FORMAT_MSA_CLUSTAL \
    | VRNA_FILE_FORMAT_MSA_STOCKHOLM \
    | VRNA_FILE_FORMAT_MSA_FASTA \
    | VRNA_FILE_FORMAT_MSA_MAF \
)
```

Option flag indicating the set of default file formats.

See also

[vrna_file_msa_read\(\)](#), [vrna_file_msa_read_record\(\)](#), [vrna_file_msa_detect_format\(\)](#)

15.59.2.6 #define VRNA_FILE_FORMAT_MSA_NOCHECK 4096U

```
#include <ViennaRNA/file_formats_msa.h>
```

Option flag to disable validation of the alignment.

See also

[vrna_file_msa_read\(\)](#), [vrna_file_msa_read_record\(\)](#)

15.59.2.7 #define VRNA_FILE_FORMAT_MSA_UNKNOWN 8192U

```
#include <ViennaRNA/file_formats_msa.h>
```

Return flag of [vrna_file_msa_detect_format\(\)](#) to indicate unknown or malformed alignment.

See also

[vrna_file_msa_detect_format\(\)](#)

15.59.3 Function Documentation

15.59.3.1 void vrna_file_helixlist (const char * seq, const char * db, float energy, FILE * file)

```
#include <ViennaRNA/file_formats.h>
```

Print a secondary structure as helix list.

Parameters

<i>seq</i>	The RNA sequence
<i>db</i>	The structure in dot-bracket format
<i>energy</i>	Free energy of the structure in kcal/mol
<i>file</i>	The file handle used to print to (print defaults to 'stdout' if(file == NULL))

15.59.3.2 int vrna_file_msa_read (const char * filename, char *** names, char *** aln, char ** id, char ** structure, unsigned int options)

```
#include <ViennaRNA/file_formats_msa.h>
```

Read a multiple sequence alignment from file.

This function reads the (first) multiple sequence alignment from an input file. The read alignment is split into the sequence id/name part and the actual sequence information and stored in memory as arrays of ids/names and sequences. If the alignment file format allows for additional information, such as an ID of the entire alignment or consensus structure information, this data is retrieved as well and made available. The `options` parameter allows to specify the set of alignment file formats that should be used to retrieve the data. If 0 is passed as option, the list of alignment file formats defaults to [VRNA_FILE_FORMAT_MSA_DEFAULT](#).

Currently, the list of parsable multiple sequence alignment file formats consists of:

- [ClustalW format](#)
- [Stockholm 1.0 format](#)
- [FASTA \(Pearson\) format](#)
- [MAF format](#)

Note

After successfully reading an alignment, this function performs a validation of the data that includes uniqueness of the sequence identifiers, and equal sequence lengths. This check can be deactivated by passing [VRNA_FILE_FORMAT_MSA_NOCHECK](#) in the `options` parameter.

See also

[vrna_file_msa_read_record\(\)](#), [VRNA_FILE_FORMAT_MSA_CLUSTAL](#), [VRNA_FILE_FORMAT_MSA_STOCKHOLM](#), [VRNA_FILE_FORMAT_MSA_FASTA](#), [VRNA_FILE_FORMAT_MSA_MAF](#), [VRNA_FILE_FORMAT_MSA_DEFAULT](#), [VRNA_FILE_FORMAT_MSA_NOCHECK](#)

Parameters

<i>filename</i>	The name of input file that contains the alignment
<i>names</i>	An address to the pointer where sequence identifiers should be written to
<i>aln</i>	An address to the pointer where aligned sequences should be written to
<i>id</i>	An address to the pointer where the alignment ID should be written to (Maybe NULL)
<i>structure</i>	An address to the pointer where consensus structure information should be written to (Maybe NULL)
<i>options</i>	Options to manipulate the behavior of this function

Returns

The number of sequences in the alignment, or -1 if no alignment record could be found

15.59.3.3 `int vrna_file_msa_read_record (FILE * fp, char *** names, char *** aln, char ** id, char ** structure, unsigned int options)`

```
#include <ViennaRNA/file_formats_msa.h>
```

Read a multiple sequence alignment from file handle.

Similar to [vrna_file_msa_read\(\)](#), this function reads a multiple sequence alignment from an input file handle. Since using a file handle, this function is not limited to the first alignment record, but allows for looping over all alignments within the input.

The read alignment is split into the sequence id/name part and the actual sequence information and stored in memory as arrays of ids/names and sequences. If the alignment file format allows for additional information, such as an ID of the entire alignment or consensus structure information, this data is retrieved as well and made available. The `options` parameter allows to specify the alignment file format used to retrieve the data. A single format must be specified here, see [vrna_file_msa_detect_format\(\)](#) for helping to determine the correct MSA file format.

Currently, the list of parsable multiple sequence alignment file formats consists of:

- [ClustalW format](#)
- [Stockholm 1.0 format](#)
- [FASTA \(Pearson\) format](#)
- [MAF format](#)

Note

After successfully reading an alignment, this function performs a validation of the data that includes uniqueness of the sequence identifiers, and equal sequence lengths. This check can be deactivated by passing [VRNA_FILE_FORMAT_MSA_NOCHECK](#) in the `options` parameter.

See also

[vrna_file_msa_read\(\)](#), [vrna_file_msa_detect_format\(\)](#), [VRNA_FILE_FORMAT_MSA_CLUSTAL](#), [VRNA_FILE_FORMAT_MSA_STOCKHOLM](#), [VRNA_FILE_FORMAT_MSA_FASTA](#), [VRNA_FILE_FORMAT_MSA_MAF](#), [VRNA_FILE_FORMAT_MSA_DEFAULT](#), [VRNA_FILE_FORMAT_MSA_NOCHECK](#)

Parameters

<i>fp</i>	The file pointer the data will be retrieved from
<i>names</i>	An address to the pointer where sequence identifiers should be written to
<i>aln</i>	An address to the pointer where aligned sequences should be written to
<i>id</i>	An address to the pointer where the alignment ID should be written to (Maybe NULL)
<i>structure</i>	An address to the pointer where consensus structure information should be written to (Maybe NULL)
<i>options</i>	Options to manipulate the behavior of this function

Returns

The number of sequences in the alignment, or -1 if no alignment record could be found

15.59.3.4 `unsigned int vrna_file_msa_detect_format (const char * filename, unsigned int options)`

```
#include <ViennaRNA/file_formats_msa.h>
```

Detect the format of a multiple sequence alignment file.

This function attempts to determine the format of a file that supposedly contains a multiple sequence alignment (MSA). This is useful in cases where a MSA file contains more than a single record and therefore [vrna_file_msa_read\(\)](#) can not be applied, since it only retrieves the first. Here, one can try to guess the correct file format using this function and then loop over the file, record by record using one of the low-level record retrieval functions for the corresponding MSA file format.

Note

This function parses the entire first record within the specified file. As a result, it returns [VRNA_FILE_FORMAT_MSA_UNKNOWN](#) not only if it can't detect the file's format, but also in cases where the file doesn't contain sequences!

See also

[vrna_file_msa_read\(\)](#), [vrna_file_stockholm_read_record\(\)](#), [vrna_file_clustal_read_record\(\)](#), [vrna_file_fasta_read_record\(\)](#)

Parameters

<i>filename</i>	The name of input file that contains the alignment
<i>options</i>	Options to manipulate the behavior of this function

Returns

The MSA file format, or [VRNA_FILE_FORMAT_MSA_UNKNOWN](#)

15.59.3.5 `char* vrna_read_line (FILE * fp)`

```
#include <ViennaRNA/file_utils.h>
```

Read a line of arbitrary length from a stream.

Returns a pointer to the resulting string. The necessary memory is allocated and should be released using *free()* when the string is no longer needed.

Parameters

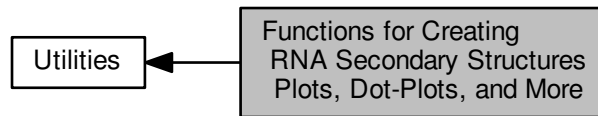
<i>fp</i>	A file pointer to the stream where the function should read from
-----------	------------------------------------------------------------------

Returns

A pointer to the resulting string

15.60 Functions for Creating RNA Secondary Structures Plots, Dot-Plots, and More

Collaboration diagram for Functions for Creating RNA Secondary Structures Plots, Dot-Plots, and More:



Files

- file [naview.h](#)
- file [plot_aln.h](#)
Various functions for plotting Sequence / Structure Alignments.
- file [plot_layouts.h](#)
Secondary structure plot layout algorithms.
- file [plot_structure.h](#)
Various functions for plotting RNA secondary structures.
- file [PS_dot.h](#)
Various functions for plotting RNA secondary structures, dot-plots and other visualizations.

- int [PS_color_aln](#) (const char *structure, const char *filename, const char *seqs[], const char *names[])
Produce PostScript sequence alignment color-annotated by consensus structure.
- int [aliPS_color_aln](#) (const char *structure, const char *filename, const char *seqs[], const char *names[])

- int [simple_xy_coordinates](#) (short *pair_table, float *X, float *Y)
Calculate nucleotide coordinates for secondary structure plot the Simple way
- int [simple_circplot_coordinates](#) (short *pair_table, float *x, float *y)
Calculate nucleotide coordinates for Circular Plot
- #define [VRNA_PLOT_TYPE_SIMPLE](#) 0
Definition of Plot type simple
- #define [VRNA_PLOT_TYPE_NAVIEW](#) 1
Definition of Plot type Naview
- #define [VRNA_PLOT_TYPE_CIRCULAR](#) 2
Definition of Plot type Circular
- int [rna_plot_type](#)
Switch for changing the secondary structure layout algorithm.

- int [vrna_file_PS_rnaplot](#) (const char *seq, const char *structure, const char *file, [vrna_md_t](#) *md_p)
Produce a secondary structure graph in PostScript and write it to 'filename'.
- int [vrna_file_PS_rnaplot_a](#) (const char *seq, const char *structure, const char *file, const char *pre, const char *post, [vrna_md_t](#) *md_p)
Produce a secondary structure graph in PostScript including additional annotation macros and write it to 'filename'.

- int [gmlRNA](#) (char *string, char *structure, char *ssfile, char option)
Produce a secondary structure graph in Graph Meta Language (gml) and write it to a file.
- int [ssv_rna_plot](#) (char *string, char *structure, char *ssfile)
Produce a secondary structure graph in SStructView format.
- int [svg_rna_plot](#) (char *string, char *structure, char *ssfile)
Produce a secondary structure plot in SVG format and write it to a file.
- int [xrna_plot](#) (char *string, char *structure, char *ssfile)
Produce a secondary structure plot for further editing in XRNA.
- int [PS_rna_plot](#) (char *string, char *structure, char *file)
Produce a secondary structure graph in PostScript and write it to 'filename'.
- int [PS_rna_plot_a](#) (char *string, char *structure, char *file, char *pre, char *post)
Produce a secondary structure graph in PostScript including additional annotation macros and write it to 'filename'.
- int [PS_rna_plot_a_gquad](#) (char *string, char *structure, char *ssfile, char *pre, char *post)
Produce a secondary structure graph in PostScript including additional annotation macros and write it to 'filename' (detect and draw g-quadruplexes)

- int [PS_dot_plot_list](#) (char *seq, char *filename, [plist](#) *pl, [plist](#) *mf, char *comment)
Produce a postscript dot-plot from two pair lists.
- int [PS_dot_plot](#) (char *string, char *file)
Produce postscript dot-plot.

15.60.1 Detailed Description

15.60.2 Macro Definition Documentation

15.60.2.1 #define VRNA_PLOT_TYPE_SIMPLE 0

```
#include <ViennaRNA/plot_layouts.h>
```

Definition of Plot type *simple*

This is the plot type definition for several RNA structure plotting functions telling them to use **Simple** plotting algorithm

See also

[rna_plot_type](#), [vrna_file_PS_rnaplot_a\(\)](#), [vrna_file_PS_rnaplot\(\)](#), [svg_rna_plot\(\)](#), [gmlRNA\(\)](#), [ssv_rna_plot\(\)](#), [xrna_plot\(\)](#)

15.60.2.2 #define VRNA_PLOT_TYPE_NAVIEW 1

```
#include <ViennaRNA/plot_layouts.h>
```

Definition of Plot type *Naview*

This is the plot type definition for several RNA structure plotting functions telling them to use **Naview** plotting algorithm

See also

[rna_plot_type](#), [vrna_file_PS_rnaplot_a\(\)](#), [vrna_file_PS_rnaplot\(\)](#), [svg_rna_plot\(\)](#), [gmlRNA\(\)](#), [ssv_rna_plot\(\)](#), [xrna_plot\(\)](#)

15.60.2.3 #define VRNA_PLOT_TYPE_CIRCULAR 2

```
#include <ViennaRNA/plot_layouts.h>
```

Definition of Plot type *Circular*

This is the plot type definition for several RNA structure plotting functions telling them to produce a **Circular plot**

See also

[rna_plot_type](#), [vrna_file_PS_rnaplot_a\(\)](#), [vrna_file_PS_rnaplot\(\)](#), [svg_rna_plot\(\)](#), [gmlRNA\(\)](#), [ssv_rna_plot\(\)](#), [xrna_plot\(\)](#)

15.60.3 Function Documentation

15.60.3.1 int aliPS_color_aln (const char * *structure*, const char * *filename*, const char * *seqs*[], const char * *names*[])

```
#include <ViennaRNA/plot_aln.h>
```

PS_color_aln for duplexes

15.60.3.2 int simple_xy_coordinates (short * *pair_table*, float * *X*, float * *Y*)

```
#include <ViennaRNA/plot_layouts.h>
```

Calculate nucleotide coordinates for secondary structure plot the *Simple way*

See also

[make_pair_table\(\)](#), [rna_plot_type](#), [simple_circplot_coordinates\(\)](#), [naview_xy_coordinates\(\)](#), [vrna_file_PS_rnaplot_a\(\)](#), [vrna_file_PS_rnaplot\(\)](#), [svg_rna_plot\(\)](#)

Parameters

<i>pair_table</i>	The pair table of the secondary structure
<i>X</i>	a pointer to an array with enough allocated space to hold the x coordinates
<i>Y</i>	a pointer to an array with enough allocated space to hold the y coordinates

Returns

length of sequence on success, 0 otherwise

15.60.3.3 int simple_circplot_coordinates (short * *pair_table*, float * *x*, float * *y*)

```
#include <ViennaRNA/plot_layouts.h>
```

Calculate nucleotide coordinates for *Circular Plot*

This function calculates the coordinates of nucleotides mapped in equal distances onto a unit circle.

Note

In order to draw nice arcs using quadratic bezier curves that connect base pairs one may calculate a second tangential point P^t in addition to the actual R^2 coordinates. the simplest way to do so may be to compute a radius scaling factor rs in the interval $[0, 1]$ that weights the proportion of base pair span to the actual length of the sequence. This scaling factor can then be used to calculate the coordinates for P^t , i.e. $P_x^t[i] = X[i] * rs$ and $P_y^t[i] = Y[i] * rs$.

See also

[make_pair_table\(\)](#), [rna_plot_type](#), [simple_xy_coordinates\(\)](#), [naview_xy_coordinates\(\)](#), [vrna_file_PS_↵
rnaplot_a\(\)](#), [vrna_file_PS_rnaplot](#), [svg_rna_plot\(\)](#)

Parameters

<i>pair_table</i>	The pair table of the secondary structure
<i>x</i>	a pointer to an array with enough allocated space to hold the x coordinates
<i>y</i>	a pointer to an array with enough allocated space to hold the y coordinates

Returns

length of sequence on success, 0 otherwise

15.60.3.4 `int vrna_file_PS_rnaplot (const char * seq, const char * structure, const char * file, vrna_md_t * md_p)`

```
#include <ViennaRNA/plot_structure.h>
```

Produce a secondary structure graph in PostScript and write it to 'filename'.

Note that this function has changed from previous versions and now expects the structure to be plotted in dot-bracket notation as an argument. It does not make use of the global [base_pair](#) array anymore.

Parameters

<i>seq</i>	The RNA sequence
<i>structure</i>	The secondary structure in dot-bracket notation
<i>file</i>	The filename of the postscript output
<i>md_p</i>	Model parameters used to generate a commandline option string in the output (Maybe NULL)

Returns

1 on success, 0 otherwise

15.60.3.5 `int vrna_file_PS_rnaplot_a (const char * seq, const char * structure, const char * file, const char * pre, const char * post, vrna_md_t * md_p)`

```
#include <ViennaRNA/plot_structure.h>
```

Produce a secondary structure graph in PostScript including additional annotation macros and write it to 'filename'.

Same as `vrna_file_PS_rnaplot()` but adds extra PostScript macros for various annotations (see generated PS code). The 'pre' and 'post' variables contain PostScript code that is verbatim copied in the resulting PS file just before and after the structure plot. If both arguments ('pre' and 'post') are NULL, no additional macros will be printed into the PostScript.

Parameters

<i>seq</i>	The RNA sequence
<i>structure</i>	The secondary structure in dot-bracket notation
<i>file</i>	The filename of the postscript output
<i>pre</i>	PostScript code to appear before the secondary structure plot
<i>post</i>	PostScript code to appear after the secondary structure plot
<i>md_p</i>	Model parameters used to generate a commandline option string in the output (Maybe NULL)

Returns

1 on success, 0 otherwise

15.60.3.6 `int gmlRNA (char * string, char * structure, char * ssfile, char option)`

```
#include <ViennaRNA/plot_structure.h>
```

Produce a secondary structure graph in Graph Meta Language (gml) and write it to a file.

If 'option' is an uppercase letter the RNA sequence is used to label nodes, if 'option' equals 'X' or 'x' the resulting file will coordinates for an initial layout of the graph.

Parameters

<i>string</i>	The RNA sequence
<i>structure</i>	The secondary structure in dot-bracket notation
<i>ssfile</i>	The filename of the gml output
<i>option</i>	The option flag

Returns

1 on success, 0 otherwise

15.60.3.7 `int ssv_rna_plot (char * string, char * structure, char * ssfile)`

```
#include <ViennaRNA/plot_structure.h>
```

Produce a secondary structure graph in SStructView format.

Write coord file for SStructView

Parameters

<i>string</i>	The RNA sequence
<i>structure</i>	The secondary structure in dot-bracket notation
<i>ssfile</i>	The filename of the ssv output

Returns

1 on success, 0 otherwise

15.60.3.8 `int svg_rna_plot (char * string, char * structure, char * ssfile)`

```
#include <ViennaRNA/plot_structure.h>
```

Produce a secondary structure plot in SVG format and write it to a file.

Parameters

<i>string</i>	The RNA sequence
<i>structure</i>	The secondary structure in dot-bracket notation
<i>ssfile</i>	The filename of the svg output

Returns

1 on success, 0 otherwise

15.60.3.9 `int xrna_plot (char * string, char * structure, char * ssfile)`

```
#include <ViennaRNA/plot_structure.h>
```

Produce a secondary structure plot for further editing in XRNA.

Parameters

<i>string</i>	The RNA sequence
<i>structure</i>	The secondary structure in dot-bracket notation
<i>ssfile</i>	The filename of the xrna output

Returns

1 on success, 0 otherwise

15.60.3.10 `int PS_rna_plot (char * string, char * structure, char * file)`

```
#include <ViennaRNA/plot_structure.h>
```

Produce a secondary structure graph in PostScript and write it to 'filename'.

Deprecated Use [vrna_file_PS_rnaplot\(\)](#) instead!

15.60.3.11 `int PS_rna_plot_a (char * string, char * structure, char * file, char * pre, char * post)`

```
#include <ViennaRNA/plot_structure.h>
```

Produce a secondary structure graph in PostScript including additional annotation macros and write it to 'filename'.

Deprecated Use [vrna_file_PS_rnaplot_a\(\)](#) instead!

15.60.3.12 `int PS_rna_plot_a_gquad (char * string, char * structure, char * ssfile, char * pre, char * post)`

```
#include <ViennaRNA/plot_structure.h>
```

Produce a secondary structure graph in PostScript including additional annotation macros and write it to 'filename' (detect and draw g-quadruplexes)

Deprecated Use [vrna_file_PS_rnaplot_a\(\)](#) instead!

15.60.3.13 `int PS_dot_plot_list (char * seq, char * filename, plist * pl, plist * mf, char * comment)`

```
#include <ViennaRNA/PS_dot.h>
```

Produce a postscript dot-plot from two pair lists.

This function reads two plist structures (e.g. base pair probabilities and a secondary structure) as produced by [assign_plist_from_pr\(\)](#) and [assign_plist_from_db\(\)](#) and produces a postscript "dot plot" that is written to 'filename'. Using base pair probabilities in the first and mfe structure in the second plist, the resulting "dot plot" represents each base pairing probability by a square of corresponding area in a upper triangle matrix. The lower part of the matrix contains the minimum free energy structure.

See also

[assign_plist_from_pr\(\)](#), [assign_plist_from_db\(\)](#)

Parameters

<i>seq</i>	The RNA sequence
<i>filename</i>	A filename for the postscript output
<i>pl</i>	The base pair probability pairlist
<i>mf</i>	The mfe secondary structure pairlist
<i>comment</i>	A comment

Returns

1 if postscript was successfully written, 0 otherwise

15.60.3.14 `int PS_dot_plot (char * string, char * file)`

```
#include <ViennaRNA/PS_dot.h>
```

Produce postscript dot-plot.

Wrapper to `PS_dot_plot_list`

Reads base pair probabilities produced by `pf_fold()` from the global array `pr` and the pair list `base_pair` produced by `fold()` and produces a postscript "dot plot" that is written to 'filename'. The "dot plot" represents each base pairing probability by a square of corresponding area in a upper triangle matrix. The lower part of the matrix contains the minimum free energy

Note

DO NOT USE THIS FUNCTION ANYMORE SINCE IT IS NOT THREADSAFE

Deprecated This function is deprecated and will be removed soon! Use `PS_dot_plot_list()` instead!

15.60.4 Variable Documentation

15.60.4.1 `int rna_plot_type`

```
#include <ViennaRNA/plot_layouts.h>
```

Switch for changing the secondary structure layout algorithm.

Current possibility are 0 for a simple radial drawing or 1 for the modified radial drawing taken from the *naview* program of [3].

Note

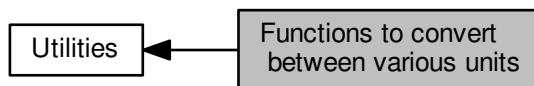
To provide thread safety please do not rely on this global variable in future implementations but pass a plot type flag directly to the function that decides which layout algorithm it may use!

See also

`VRNA_PLOT_TYPE_SIMPLE`, `VRNA_PLOT_TYPE_NAVIEW`, `VRNA_PLOT_TYPE_CIRCULAR`

15.61 Functions to convert between various units

Collaboration diagram for Functions to convert between various units:



Files

- file [units.h](#)
Physical Units and Functions to convert them into each other.
- double [vrna_convert_energy](#) (double energy, [vrna_unit_energy_e](#) from, [vrna_unit_energy_e](#) to)
Convert between energy / work units.
- double [vrna_convert_temperature](#) (double temp, [vrna_unit_temperature_e](#) from, [vrna_unit_temperature_e](#) to)
Convert between temperature units.

15.61.1 Detailed Description

15.61.2 Enumeration Type Documentation

15.61.2.1 enum [vrna_unit_energy_e](#)

```
#include <ViennaRNA/units.h>
```

Energy / Work Units.

See also

[vrna_convert_energy\(\)](#)

Enumerator

VRNA_UNIT_J Joule ($1\text{ J} = 1\text{ kg} \cdot \text{m}^2 \text{s}^{-2}$)
VRNA_UNIT_KJ Kilojoule ($1\text{ kJ} = 1,000\text{ J}$)
VRNA_UNIT_CAL_IT Calorie (International (Steam) Table, $1\text{ cal}_{IT} = 4.1868\text{ J}$)
VRNA_UNIT_DACAL_IT Decacalorie (International (Steam) Table, $1\text{ dacal}_{IT} = 10\text{ cal}_{IT} = 41.868\text{ J}$)
VRNA_UNIT_KCAL_IT Kilocalorie (International (Steam) Table, $1\text{ kcal}_{IT} = 4.1868\text{ kJ}$)
VRNA_UNIT_CAL Calorie (Thermochemical, $1\text{ cal}_{th} = 4.184\text{ J}$)
VRNA_UNIT_DACAL Decacalorie (Thermochemical, $1\text{ dacal}_{th} = 10\text{ cal}_{th} = 41.84\text{ J}$)
VRNA_UNIT_KCAL Kilocalorie (Thermochemical, $1\text{ kcal}_{th} = 4.184\text{ kJ}$)
VRNA_UNIT_G_TNT g TNT ($1\text{ g TNT} = 1,000\text{ cal}_{th} = 4,184\text{ J}$)
VRNA_UNIT_KG_TNT kg TNT ($1\text{ kg TNT} = 1,000\text{ kcal}_{th} = 4,184\text{ kJ}$)
VRNA_UNIT_T_TNT ton TNT ($1\text{ t TNT} = 1,000,000\text{ kcal}_{th} = 4,184\text{ MJ}$)
VRNA_UNIT_EV Electronvolt ($1\text{ eV} = 1.602176565 \times 10^{-19}\text{ J}$)
VRNA_UNIT_WH Watt hour ($1\text{ W} \cdot \text{h} = 1\text{ W} \cdot 3,600\text{ s} = 3,600\text{ J} = 3.6\text{ kJ}$)
VRNA_UNIT_KWH Kilowatt hour ($1\text{ kW} \cdot \text{h} = 1\text{ kW} \cdot 3,600\text{ s} = 3,600\text{ kJ} = 3.6\text{ MJ}$)

15.61.2.2 enum vrna_unit_temperature_e

```
#include <ViennaRNA/units.h>
```

Temperature Units.

See also

[vrna_convert_temperature\(\)](#)

Enumerator

VRNA_UNIT_K Kelvin (K)

VRNA_UNIT_DEG_C Degree Celcius (°C) ($[^{\circ}C] = [K] - 273.15$)

VRNA_UNIT_DEG_F Degree Fahrenheit (°F) ($[^{\circ}F] = [K] \times \frac{9}{5} - 459.67$)

VRNA_UNIT_DEG_R Degree Rankine (°R) ($[^{\circ}R] = [K] \times \frac{9}{5}$)

VRNA_UNIT_DEG_N Degree Newton (°N) ($[^{\circ}N] = ([K] - 273.15) \times \frac{33}{100}$)

VRNA_UNIT_DEG_DE Degree Delisle (°De) ($[^{\circ}De] = (373.15 - [K]) \frac{3}{2}$)

VRNA_UNIT_DEG_RE Degree Réaumur (°Ré) ($[^{\circ}Ré] = ([K] - 273.15) \times \frac{4}{5}$)

VRNA_UNIT_DEG_RO Degree Rømer (°Rø) ($[^{\circ}R] = ([K] - 273.15) \times \frac{21}{40} + 7.5$)

15.61.3 Function Documentation

15.61.3.1 double vrna_convert_energy (double energy, vrna_unit_energy_e from, vrna_unit_energy_e to)

```
#include <ViennaRNA/units.h>
```

Convert between energy / work units.

See also

[vrna_unit_energy_e](#)

Parameters

<i>energy</i>	Input energy value
<i>from</i>	Input unit
<i>to</i>	Output unit

Returns

Energy value in Output unit

15.61.3.2 double vrna_convert_temperature (double temp, vrna_unit_temperature_e from, vrna_unit_temperature_e to)

```
#include <ViennaRNA/units.h>
```

Convert between temperature units.

See also

[vrna_unit_temperature_e](#)

Parameters

<i>temp</i>	Input temperature value
<i>from</i>	Input unit
<i>to</i>	Output unit

Returns

Temperature value in Output unit

Chapter 16

Data Structure Documentation

16.1 `_struct_en` Struct Reference

Data structure for [energy_of_move\(\)](#)

16.1.1 Detailed Description

Data structure for [energy_of_move\(\)](#)

The documentation for this struct was generated from the following file:

- ViennaRNA/move_set.h

16.2 `COORDINATE` Struct Reference

this is a workaround for the SWIG Perl Wrapper RNA plot function that returns an array of type [COORDINATE](#)

16.2.1 Detailed Description

this is a workaround for the SWIG Perl Wrapper RNA plot function that returns an array of type [COORDINATE](#)

The documentation for this struct was generated from the following file:

- ViennaRNA/[plot_layouts.h](#)

16.3 `Postorder_list` Struct Reference

Postorder data structure.

16.3.1 Detailed Description

Postorder data structure.

The documentation for this struct was generated from the following file:

- ViennaRNA/[dist_vars.h](#)

16.4 swString Struct Reference

Some other data structure.

16.4.1 Detailed Description

Some other data structure.

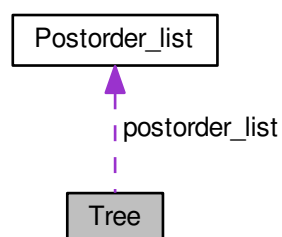
The documentation for this struct was generated from the following file:

- ViennaRNA/[dist_vars.h](#)

16.5 Tree Struct Reference

[Tree](#) data structure.

Collaboration diagram for Tree:



16.5.1 Detailed Description

[Tree](#) data structure.

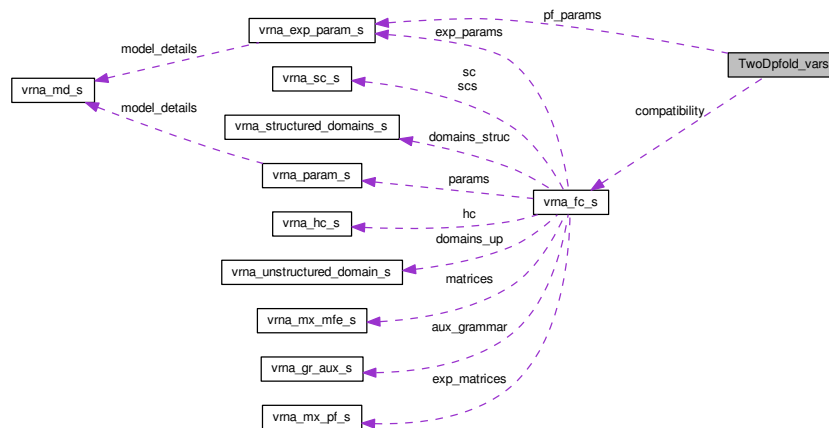
The documentation for this struct was generated from the following file:

- ViennaRNA/[dist_vars.h](#)

16.6 TwoDpfold_vars Struct Reference

Variables compound for 2Dfold partition function folding.

Collaboration diagram for TwoDpfold_vars:



Data Fields

- char * [ptype](#)
Precomputed array of pair types.
- char * [sequence](#)
The input sequence.
- short * [S1](#)
The input sequences in numeric form.
- unsigned int [maxD1](#)
Maximum allowed base pair distance to first reference.
- unsigned int [maxD2](#)
Maximum allowed base pair distance to second reference.
- int * [my_iindx](#)
Index for moving in quadratic distance dimensions.
- int * [jindx](#)
Index for moving in the triangular matrix qm1.
- unsigned int * [referenceBPs1](#)
Matrix containing number of basepairs of reference structure1 in interval [i,j].
- unsigned int * [referenceBPs2](#)
Matrix containing number of basepairs of reference structure2 in interval [i,j].
- unsigned int * [bpdist](#)
Matrix containing base pair distance of reference structure 1 and 2 on interval [i,j].
- unsigned int * [mm1](#)
Maximum matching matrix, reference struct 1 disallowed.
- unsigned int * [mm2](#)
Maximum matching matrix, reference struct 2 disallowed.

16.6.1 Detailed Description

Variables compound for 2Dfold partition function folding.

Deprecated This data structure will be removed from the library soon! Use [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_pf_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

The documentation for this struct was generated from the following file:

- [ViennaRNA/2Dpfold.h](#)

16.7 vrna_command_s Struct Reference

List element for commands ready for application to a [vrna_fold_compound_t](#).

16.7.1 Detailed Description

List element for commands ready for application to a [vrna_fold_compound_t](#).

See also

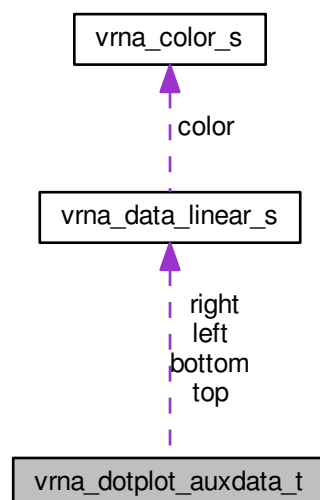
[vrna_file_commands_read\(\)](#), [vrna_commands_apply\(\)](#), [vrna_commands_free\(\)](#)

The documentation for this struct was generated from the following file:

- [ViennaRNA/commands.h](#)

16.8 vrna_dotplot_auxdata_t Struct Reference

Collaboration diagram for [vrna_dotplot_auxdata_t](#):



The documentation for this struct was generated from the following file:

- [ViennaRNA/PS_dot.h](#)

16.9 vrna_gr_aux_s Struct Reference

The documentation for this struct was generated from the following file:

- [ViennaRNA/grammar.h](#)

16.10 vrna_hx_s Struct Reference

Data structure representing an entry of a helix list.

16.10.1 Detailed Description

Data structure representing an entry of a helix list.

The documentation for this struct was generated from the following file:

- [ViennaRNA/structure_utils.h](#)

16.11 vrna_md_s Struct Reference

The data structure that contains the complete model details used throughout the calculations.

Data Fields

- double [temperature](#)
The temperature used to scale the thermodynamic parameters.
- double [betaScale](#)
A scaling factor for the thermodynamic temperature of the Boltzmann factors.
- int [dangles](#)
Specifies the dangle model used in any energy evaluation (0,1,2 or 3)
- int [special_hp](#)
Include special hairpin contributions for tri, tetra and hexaloops.
- int [noLP](#)
Only consider canonical structures, i.e. no 'lonely' base pairs.
- int [noGU](#)
Do not allow GU pairs.
- int [noGUclosure](#)
Do not allow loops to be closed by GU pair.
- int [logML](#)
Use logarithmic scaling for multiloops.
- int [circ](#)

- *Assume RNA to be circular instead of linear.*
- int `gquad`
Include G-quadruplexes in structure prediction.
- int `canonicalBPonly`
remove non-canonical bp's from constraint structures
- int `uniq_ML`
Flag to ensure unique multi-branch loop decomposition during folding.
- int `energy_set`
Specifies the energy set that defines set of compatible base pairs.
- int `backtrack`
Specifies whether or not secondary structures should be backtraced.
- char `backtrack_type`
Specifies in which matrix to backtrack.
- int `compute_bpp`
Specifies whether or not backward recursions for base pair probability (bpp) computation will be performed.
- char `nonstandards` [64]
contains allowed non standard bases
- int `max_bp_span`
maximum allowed base pair span
- int `min_loop_size`
Minimum size of hairpin loops.
- int `window_size`
Size of the sliding window for locally optimal structure prediction.
- int `oldAliEn`
Use old alifold energy model.
- int `ribo`
Use ribosum scoring table in alifold energy model.
- double `cv_fact`
Co-variance scaling factor for consensus structure prediction.
- double `nc_fact`
Scaling factor to weight co-variance contributions of non-canonical pairs.
- double `sfact`
Scaling factor for partition function scaling.
- int `rtype` [8]
Reverse base pair type array.
- short `alias` [MAXALPHA+1]
alias of an integer nucleotide representation
- int `pair` [MAXALPHA+1][MAXALPHA+1]
Integer representation of a base pair.

16.11.1 Detailed Description

The data structure that contains the complete model details used throughout the calculations.

For convenience reasons, we provide the type name `vrna_md_t` to address this data structure without the use of the struct keyword

See also

[vrna_md_set_default\(\)](#), [set_model_details\(\)](#), [vrna_md_update\(\)](#), [vrna_md_t](#)

SWIG Wrapper Notes This data structure is wrapped as an object **md** with multiple related functions attached as methods.

A new set of default parameters can be obtained by calling the constructor of **md**:

- *md()* – Initialize with default settings

The resulting object has a list of attached methods which directly correspond to functions that mainly operate on the corresponding C data structure:

- *reset()* – [vrna_md_set_default\(\)](#)
- *set_from_globals()* – [set_model_details\(\)](#)
- *option_string()* – [vrna_md_option_string\(\)](#)

Note, that default parameters can be modified by directly setting any of the following global variables. Internally, getting/setting default parameters using their global variable representative translates into calls of the following functions, therefore these wrappers for these functions do not exist in the scripting language interface(s):

global variable	C getter	C setter
temperature	vrna_md_defaults_↔ temperature_get()	vrna_md_defaults_↔ temperature()
dangles	vrna_md_defaults_dangles_↔ get()	vrna_md_defaults_dangles()
betaScale	vrna_md_defaults_betaScale↔ _get()	vrna_md_defaults_betaScale()
tetra_loop	this is an alias of <i>special_hp</i>	
special_hp	vrna_md_defaults_special_hp↔ _get()	vrna_md_defaults_special_hp()
noLonelyPairs	this is an alias of <i>noLP</i>	
noLP	vrna_md_defaults_noLP_get()	vrna_md_defaults_noLP()
noGU	vrna_md_defaults_noGU_get()	vrna_md_defaults_noGU()
no_closingGU	this is an alias of <i>noGUclosure</i>	
noGUclosure	vrna_md_defaults_noG↔ Uclosure_get()	vrna_md_defaults_noG↔ Uclosure()
logML	vrna_md_defaults_logML_get()	vrna_md_defaults_logML()
circ	vrna_md_defaults_circ_get()	vrna_md_defaults_circ()
gquad	vrna_md_defaults_gquad_get()	vrna_md_defaults_gquad()
uniq_ML	vrna_md_defaults_uniq_ML_↔ get()	vrna_md_defaults_uniq_ML()
energy_set	vrna_md_defaults_energy_↔ set_get()	vrna_md_defaults_energy_set()
backtrack	vrna_md_defaults_backtrack_↔ get()	vrna_md_defaults_backtrack()
backtrack_type	vrna_md_defaults_backtrack_↔ type_get()	vrna_md_defaults_backtrack_↔ type()
do_backtrack	this is an alias of <i>compute_bpp</i>	
compute_bpp	vrna_md_defaults_compute_↔ bpp_get()	vrna_md_defaults_compute_↔ bpp()

global variable	C getter	C setter
max_bp_span	vrna_md_defaults_max_bp_↔span_get()	vrna_md_defaults_max_bp_↔span()
min_loop_size	vrna_md_defaults_min_loop_↔size_get()	vrna_md_defaults_min_loop_↔size()
window_size	vrna_md_defaults_window_↔size_get()	vrna_md_defaults_window_↔size()
oldAliEn	vrna_md_defaults_oldAliEn_↔get()	vrna_md_defaults_oldAliEn()
ribo	vrna_md_defaults_ribo_get()	vrna_md_defaults_ribo()
cv_fact	vrna_md_defaults_cv_fact_get()	vrna_md_defaults_cv_fact()
nc_fact	vrna_md_defaults_nc_fact_get()	vrna_md_defaults_nc_fact()
sfact	vrna_md_defaults_sfact_get()	vrna_md_defaults_sfact()

16.11.2 Field Documentation

16.11.2.1 int vrna_md_s::dangles

Specifies the dangle model used in any energy evaluation (0,1,2 or 3)

If set to 0 no stabilizing energies are assigned to bases adjacent to helices in free ends and multiloops (so called dangling ends). Normally (dangles = 1) dangling end energies are assigned only to unpaired bases and a base cannot participate simultaneously in two dangling ends. In the partition function algorithm [vrna_pf\(\)](#) these checks are neglected. To provide comparability between free energy minimization and partition function algorithms, the default setting is 2. This treatment of dangling ends gives more favorable energies to helices directly adjacent to one another, which can be beneficial since such helices often do engage in stabilizing interactions through co-axial stacking.

If set to 3 co-axial stacking is explicitly included for adjacent helices in multiloops. The option affects only mfe folding and energy evaluation ([vrna_mfe\(\)](#) and [vrna_eval_structure\(\)](#)), as well as suboptimal folding ([vrna_subopt\(\)](#)) via re-evaluation of energies. Co-axial stacking with one intervening mismatch is not considered so far.

Note

Some function do not implement all dangle model but only a subset of (0,1,2,3). In particular, partition function algorithms can only handle 0 and 2. Read the documentation of the particular recurrences or energy evaluation function for information about the provided dangle model.

16.11.2.2 int vrna_md_s::min_loop_size

Minimum size of hairpin loops.

Note

The default value for this field is [TURN](#), however, it may be 0 in cofolding context.

The documentation for this struct was generated from the following file:

- [ViennaRNA/model.h](#)

16.12 vrna_pinfo_s Struct Reference

A base pair info structure.

Data Fields

- unsigned [i](#)
nucleotide position i
- unsigned [j](#)
nucleotide position j
- float [p](#)
Probability.
- float [ent](#)
*Pseudo entropy for $p(i, j) = S_i + S_j - p_{ij} * \ln(p_{ij})$.*
- short [bp](#) [8]
Frequencies of pair_types.
- char [comp](#)
1 iff pair is in mfe structure

16.12.1 Detailed Description

A base pair info structure.

For each base pair (i,j) with i,j in [0, n-1] the structure lists:

- its probability 'p'
- an entropy-like measure for its well-definedness 'ent'
- the frequency of each type of pair in 'bp[]'
 - 'bp[0]' contains the number of non-compatible sequences
 - 'bp[1]' the number of CG pairs, etc.

The documentation for this struct was generated from the following file:

- ViennaRNA/[aln_util.h](#)

16.13 vrna_sc_motif_s Struct Reference

The documentation for this struct was generated from the following file:

- ViennaRNA/[constraints_ligand.h](#)

16.14 vrna_structured_domains_s Struct Reference

The documentation for this struct was generated from the following file:

- ViennaRNA/[structured_domains.h](#)

16.15 vrna_subopt_sol_s Struct Reference

Solution element from subopt.c.

Data Fields

- float [energy](#)
Free Energy of structure in kcal/mol.
- char * [structure](#)
Structure in dot-bracket notation.

16.15.1 Detailed Description

Solution element from subopt.c.

The documentation for this struct was generated from the following file:

- ViennaRNA/[subopt.h](#)

16.16 vrna_unstructured_domain_motif_s Struct Reference

The documentation for this struct was generated from the following file:

- ViennaRNA/[unstructured_domains.h](#)

Chapter 17

File Documentation

17.1 ViennaRNA/1.8.4_epars.h File Reference

Free energy parameters for parameter file conversion.

17.1.1 Detailed Description

Free energy parameters for parameter file conversion.

This file contains the free energy parameters used in ViennaRNAPackage 1.8.4. They are summarized in:

D.H.Mathews, J. Sabina, M. ZUker, D.H. Turner "Expanded sequence dependence of thermodynamic parameters improves prediction of RNA secondary structure" JMB, 288, pp 911-940, 1999

Enthalpies taken from:

A. Walter, D Turner, J Kim, M Lyttle, P M"uller, D Mathews, M Zuker "Coaxial stckaing of helices enhances binding of oligoribonucleotides.." PNAS, 91, pp 9218-9222, 1994

D.H. Turner, N. Sugimoto, and S.M. Freier. "RNA Structure Prediction", Ann. Rev. Biophys. Biophys. Chem. 17, 167-192, 1988.

John A.Jaeger, Douglas H.Turner, and Michael Zuker. "Improved predictions of secondary structures for RNA", PNAS, 86, 7706-7710, October 1989.

L. He, R. Kierzek, J. SantaLucia, A.E. Walter, D.H. Turner "Nearest-Neughbor Parameters for GU Mismatches...." Biochemistry 1991, 30 11124-11132

A.E. Peritz, R. Kierzek, N, Sugimoto, D.H. Turner "Thermodynamic Study of Internal Loops in Oligoribonucleotides..." Biochemistry 1991, 30, 6428-6435

17.2 ViennaRNA/1.8.4_intloops.h File Reference

Free energy parameters for interior loop contributions needed by the parameter file conversion functions.

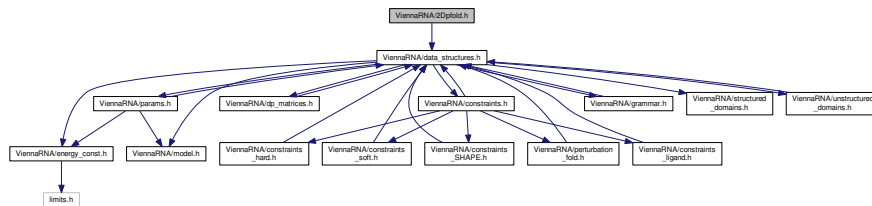
17.3.1 Detailed Description

MFE structures for base pair distance classes.

17.4 ViennaRNA/2Dpfold.h File Reference

Partition function implementations for base pair distance classes.

Include dependency graph for 2Dpfold.h:



Data Structures

- struct [vrna_sol_TwoD_pf_t](#)
Solution element returned from [vrna_pf_TwoD\(\)](#) [More...](#)
- struct [TwoDpfold_vars](#)
Variables compound for 2Dfold partition function folding.

Typedefs

- typedef struct [vrna_sol_TwoD_pf_t](#) [vrna_sol_TwoD_pf_t](#)
Solution element returned from [vrna_pf_TwoD\(\)](#)

Functions

- [vrna_sol_TwoD_pf_t](#) * [vrna_pf_TwoD](#) ([vrna_fold_compound_t](#) *vc, int maxDistance1, int maxDistance2)
Compute the partition function for all distance classes.
- char * [vrna_pbacktrack_TwoD](#) ([vrna_fold_compound_t](#) *vc, int d1, int d2)
Sample secondary structure representatives from a set of distance classes according to their Boltzmann probability.
- char * [vrna_pbacktrack5_TwoD](#) ([vrna_fold_compound_t](#) *vc, int d1, int d2, unsigned int length)
Sample secondary structure representatives with a specified length from a set of distance classes according to their Boltzmann probability.
- [TwoDpfold_vars](#) * [get_TwoDpfold_variables](#) (const char *seq, const char *structure1, char *structure2, int circ)
Get a datastructure containing all necessary attributes and global folding switches.
- void [destroy_TwoDpfold_variables](#) ([TwoDpfold_vars](#) *vars)
Free all memory occupied by a [TwoDpfold_vars](#) datastructure.
- [vrna_sol_TwoD_pf_t](#) * [TwoDpfoldList](#) ([TwoDpfold_vars](#) *vars, int maxDistance1, int maxDistance2)
Compute the partition function for all distance classes.
- char * [TwoDpfold_pbacktrack](#) ([TwoDpfold_vars](#) *vars, int d1, int d2)
Sample secondary structure representatives from a set of distance classes according to their Boltzmann probability.
- char * [TwoDpfold_pbacktrack5](#) ([TwoDpfold_vars](#) *vars, int d1, int d2, unsigned int length)
Sample secondary structure representatives with a specified length from a set of distance classes according to their Boltzmann probability.

17.4.1 Detailed Description

Partition function implementations for base pair distance classes.

17.4.2 Function Documentation

17.4.2.1 `TwoDpfold_vars* get_TwoDpfold_variables (const char * seq, const char * structure1, char * structure2, int circ)`

Get a datastructure containing all necessary attributes and global folding switches.

This function prepares all necessary attributes and matrices etc which are needed for a call of `TwoDpfold()`. A snapshot of all current global model switches (dangles, temperature and so on) is done and stored in the returned datastructure. Additionally, all matrices that will hold the partition function values are prepared.

Deprecated Use the new API that relies on `vrna_fold_compound_t` and the corresponding functions `vrna_fold_compound_TwoD()`, `vrna_pf_TwoD()`, and `vrna_fold_compound_free()` instead!

Parameters

<i>seq</i>	the RNA sequence in uppercase format with letters from the alphabet {AUCG}
<i>structure1</i>	the first reference structure in dot-bracket notation
<i>structure2</i>	the second reference structure in dot-bracket notation
<i>circ</i>	a switch indicating if the sequence is linear (0) or circular (1)

Returns

the datastructure containing all necessary partition function attributes

17.4.2.2 `void destroy_TwoDpfold_variables (TwoDpfold_vars * vars)`

Free all memory occupied by a `TwoDpfold_vars` datastructure.

This function free's all memory occupied by a datastructure obtained from `get_TwoDpfold_variables()` or `get_TwoDpfold_variables_from_MFE()`

Deprecated Use the new API that relies on `vrna_fold_compound_t` and the corresponding functions `vrna_fold_compound_TwoD()`, `vrna_pf_TwoD()`, and `vrna_fold_compound_free()` instead!

See also

`get_TwoDpfold_variables()`, `get_TwoDpfold_variables_from_MFE()`

Parameters

<i>vars</i>	the datastructure to be free'd
-------------	--------------------------------

17.4.2.3 `vrna_sol_TwoD_pf_t* TwoDpfoldList (TwoDpfold_vars * vars, int maxDistance1, int maxDistance2)`

Compute the partition function for all distance classes.

This function computes the partition functions for all distance classes according the two reference structures specified in the datastructure 'vars'. Similar to `TwoDfold()` the arguments `maxDistance1` and `maxDistance2` specify the maximum distance to both reference structures. A value of `-1` in either of them makes the appropriate distance restrictionless, i.e. all basepair distances to the reference are taken into account during computation. In case there is a restriction, the returned solution contains an entry where the attribute `k=-1` contains the partition function for all structures exceeding the restriction. A values of `INF` in the attribute 'k' of the returned list denotes the end of the list

Deprecated Use the new API that relies on `vrna_fold_compound_t` and the corresponding functions `vrna_fold_compound_TwoD()`, `vrna_pf_TwoD()`, and `vrna_fold_compound_free()` instead!

See also

[get_TwoDpfold_variables\(\)](#), [destroy_TwoDpfold_variables\(\)](#), [vrna_sol_TwoD_pf_t](#)

Parameters

<i>vars</i>	the datastructure containing all necessary folding attributes and matrices
<i>maxDistance1</i>	the maximum basepair distance to reference1 (may be -1)
<i>maxDistance2</i>	the maximum basepair distance to reference2 (may be -1)

Returns

a list of partition funtions for the appropriate distance classes

17.4.2.4 `char* TwoDpfold_pbacktrack (TwoDpfold_vars * vars, int d1, int d2)`

Sample secondary structure representatives from a set of distance classes according to their Boltzmann probability.

If the argument 'd1' is set to `-1`, the structure will be backtracked in the distance class where all structures exceeding the maximum basepair distance to either of the references reside.

Precondition

The argument 'vars' must contain precalculated partition function matrices, i.e. a call to `TwoDpfold()` preceding this function is mandatory!

Deprecated Use the new API that relies on `vrna_fold_compound_t` and the corresponding functions `vrna_fold_compound_TwoD()`, `vrna_pf_TwoD()`, `vrna_pbacktrack_TwoD()`, and `vrna_fold_compound_free()` instead!

See also

`TwoDpfold()`

Parameters

in	<i>vars</i>	the datastructure containing all necessary folding attributes and matrices
in	<i>d1</i>	the distance to reference1 (may be -1)
in	<i>d2</i>	the distance to reference2

Returns

A sampled secondary structure in dot-bracket notation

17.4.2.5 `char* TwoDpfold_pbacktrack5 (TwoDpfold_vars * vars, int d1, int d2, unsigned int length)`

Sample secondary structure representatives with a specified length from a set of distance classes according to their Boltzmann probability.

This function does essentially the same as [TwoDpfold_pbacktrack\(\)](#) with the only difference that partial structures, i.e. structures beginning from the 5' end with a specified length of the sequence, are backtracked

Note

This function does not work (since it makes no sense) for circular RNA sequences!

Precondition

The argument 'vars' must contain precalculated partition function matrices, i.e. a call to [TwoDpfold\(\)](#) preceding this function is mandatory!

Deprecated Use the new API that relies on [vrna_fold_compound_t](#) and the corresponding functions [vrna_fold_compound_TwoD\(\)](#), [vrna_pf_TwoD\(\)](#), [vrna_pbacktrack5_TwoD\(\)](#), and [vrna_fold_compound_free\(\)](#) instead!

See also

[TwoDpfold_pbacktrack\(\)](#), [TwoDpfold\(\)](#)

Parameters

in	<i>vars</i>	the datastructure containing all necessary folding attributes and matrices
in	<i>d1</i>	the distance to reference1 (may be -1)
in	<i>d2</i>	the distance to reference2
in	<i>length</i>	the length of the structure beginning from the 5' end

Returns

A sampled secondary structure in dot-bracket notation

Sample a consensus secondary structure from the Boltzmann ensemble according its probability.

- int [get_alipf_arrays](#) (short ***S_p, short ***S5_p, short ***S3_p, unsigned short ***a2s_p, char ***Ss↔_p, [FLT_OR_DBL](#) **qb_p, [FLT_OR_DBL](#) **qm_p, [FLT_OR_DBL](#) **q1k_p, [FLT_OR_DBL](#) **qIn_p, short **pscore)

Get pointers to (almost) all relevant arrays used in alifold's partition function computation.

- void [update_alifold_params](#) (void)

Update the energy parameters for alifold function.

Variables

- double [cv_fact](#)

This variable controls the weight of the covariance term in the energy function of alignment folding algorithms.

- double [nc_fact](#)

This variable controls the magnitude of the penalty for non-compatible sequences in the covariance term of alignment folding algorithms.

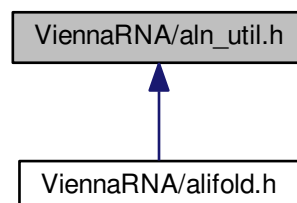
17.5.1 Detailed Description

Functions for comparative structure prediction using RNA sequence alignments.

17.6 ViennaRNA/aln_util.h File Reference

Various utility- and helper-functions for sequence alignments and comparative structure prediction.

This graph shows which files directly or indirectly include this file:



Data Structures

- struct [vrna_pinfo_s](#)

A base pair info structure.

- typedef struct [vrna_pinfo_s](#) [vrna_pinfo_t](#)

Typename for the base pair info representing data structure [vrna_pinfo_s](#).

- typedef struct [vrna_pinfo_s](#) [pair_info](#)

- Old typename of [vrna_pinfo_s](#).

 - int [vrna_aln_mpi](#) (const char **alignment)

Get the mean pairwise identity in steps from ?to?(ident)

 - [vrna_pinfo_t](#) * [vrna_aln_pinfo](#) ([vrna_fold_compound_t](#) *vc, const char *structure, double threshold)
- Retrieve an array of [vrna_pinfo_t](#) structures from precomputed pair probabilities.
- int [get_mpi](#) (char *Aseq[], int n_seq, int length, int *mini)
- Get the mean pairwise identity in steps from ?to?(ident)
- void [encode_aln_sequence](#) (const char *sequence, short *S, short *s5, short *s3, char *ss, unsigned short *as, int circ)
- Get arrays with encoded sequence of the alignment.
- void [alloc_sequence_arrays](#) (const char **sequences, short ***S, short ***S5, short ***S3, unsigned short ***a2s, char ***Ss, int circ)
- Allocate memory for sequence array used to deal with aligned sequences.
- void [free_sequence_arrays](#) (unsigned int n_seq, short ***S, short ***S5, short ***S3, unsigned short ***a2s, char ***Ss)
- Free the memory of the sequence arrays used to deal with aligned sequences.

17.6.1 Detailed Description

Various utility- and helper-functions for sequence alignments and comparative structure prediction.

17.6.2 Typedef Documentation

17.6.2.1 typedef struct vrna_pinfo_s pair_info

Old typename of [vrna_pinfo_s](#).

Deprecated Use [vrna_pinfo_t](#) instead!

17.6.3 Function Documentation

17.6.3.1 [vrna_pinfo_t](#)* [vrna_aln_pinfo](#) ([vrna_fold_compound_t](#) * vc, const char * structure, double threshold)

Retrieve an array of [vrna_pinfo_t](#) structures from precomputed pair probabilities.

This array of structures contains information about positionwise pair probabilities, base pair entropy and more

See also

[vrna_pinfo_t](#), and [vrna_pf\(\)](#)

Parameters

<i>vc</i>	The vrna_fold_compound_t of type VRNA_FC_TYPE_COMPARATIVE with precomputed partition function matrices
<i>structure</i>	An optional structure in dot-bracket notation (Maybe NULL)
<i>threshold</i>	Do not include results with pair probabilities below threshold

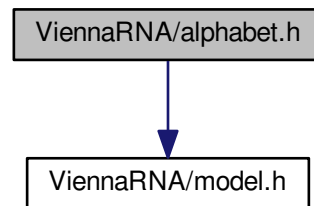
Returns

The `vrna_pinfo_t` array

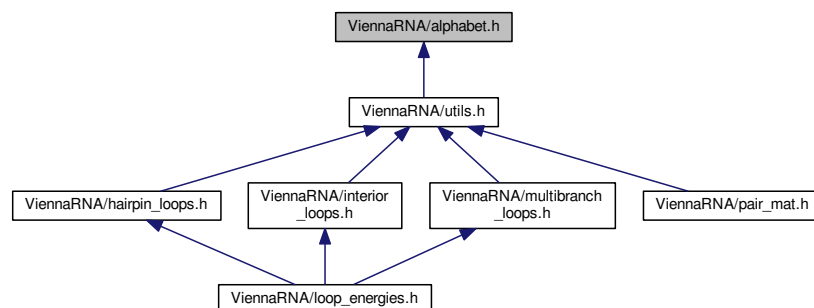
17.7 ViennaRNA/alphabet.h File Reference

Functions to process, convert, and generally handle different nucleotide and/or base pair alphabets.

Include dependency graph for alphabet.h:



This graph shows which files directly or indirectly include this file:



Functions

- char * `vrna_ptypes` (const short *S, `vrna_md_t` *md)
Get an array of the numerical encoding for each possible base pair (i,j)
- short * `vrna_seq_encode` (const char *sequence, `vrna_md_t` *md)
Get a numerical representation of the nucleotide sequence.
- short * `vrna_seq_encode_simple` (const char *sequence, `vrna_md_t` *md)
Get a numerical representation of the nucleotide sequence (simple version)
- int `vrna_nucleotide_encode` (char c, `vrna_md_t` *md)
Encode a nucleotide character to numerical value.
- char `vrna_nucleotide_decode` (int enc, `vrna_md_t` *md)
Decode a numerical representation of a nucleotide back into nucleotide alphabet.

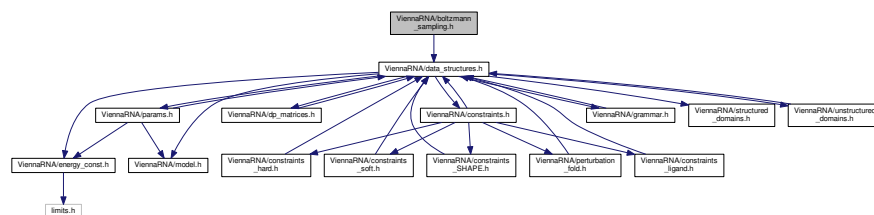
17.7.1 Detailed Description

Functions to process, convert, and generally handle different nucleotide and/or base pair alphabets.

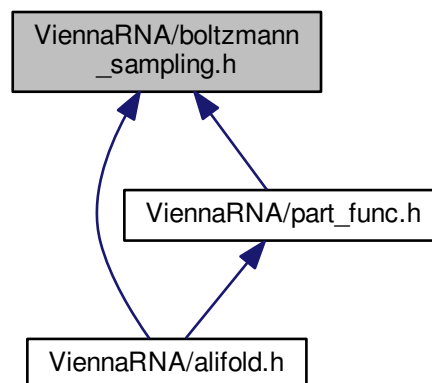
17.8 ViennaRNA/boltzmann_sampling.h File Reference

Boltzmann Sampling of secondary structures from the ensemble.

Include dependency graph for boltzmann_sampling.h:



This graph shows which files directly or indirectly include this file:



Functions

- char * [vrna_pbacktrack5](#) ([vrna_fold_compound_t](#) *vc, int length)
Sample a secondary structure of a subsequence from the Boltzmann ensemble according its probability.
- char * [vrna_pbacktrack](#) ([vrna_fold_compound_t](#) *vc)
Sample a secondary structure (consensus structure) from the Boltzmann ensemble according its probability.

17.8.1 Detailed Description

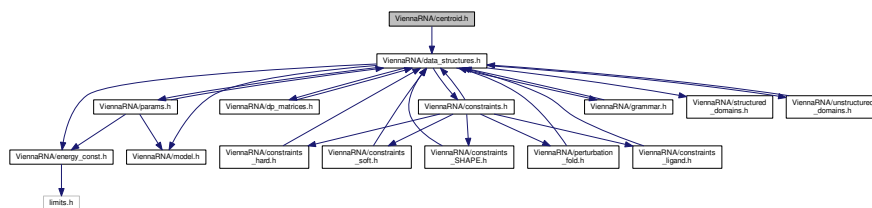
Boltzmann Sampling of secondary structures from the ensemble.

A.k.a. Stochastic backtracking

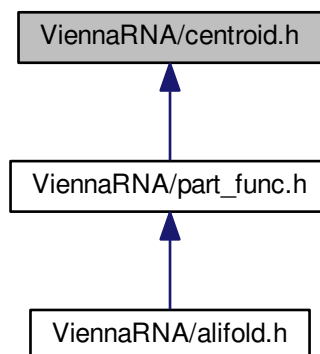
17.9 ViennaRNA/centroid.h File Reference

Centroid structure computation.

Include dependency graph for centroid.h:



This graph shows which files directly or indirectly include this file:



Functions

- char * [vrna_centroid](#) (vrna_fold_compound_t *vc, double *dist)
Get the centroid structure of the ensemble.
- char * [vrna_centroid_from_plist](#) (int length, double *dist, vrna_plist_t *pl)
Get the centroid structure of the ensemble.
- char * [vrna_centroid_from_probs](#) (int length, double *dist, FLT_OR_DBL *probs)
Get the centroid structure of the ensemble.
- char * [get_centroid_struct_pl](#) (int length, double *dist, vrna_plist_t *pl)
Get the centroid structure of the ensemble.
- char * [get_centroid_struct_pr](#) (int length, double *dist, FLT_OR_DBL *pr)
Get the centroid structure of the ensemble.

17.9.1 Detailed Description

Centroid structure computation.

17.9.2 Function Documentation

17.9.2.1 `char* get_centroid_struct_pl (int length, double * dist, vrna_plist_t * pl)`

Get the centroid structure of the ensemble.

Deprecated This function was renamed to `vrna_centroid_from_plist()`

17.9.2.2 `char* get_centroid_struct_pr (int length, double * dist, FLT_OR_DBL * pr)`

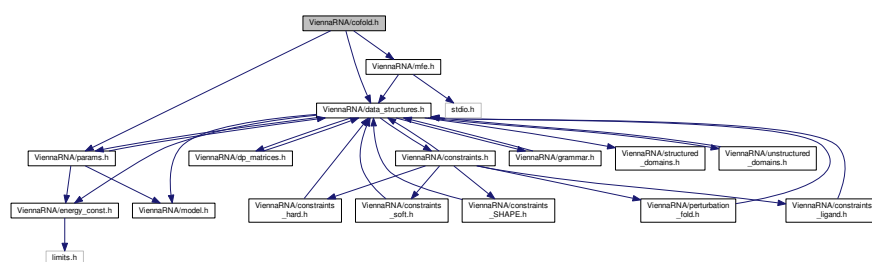
Get the centroid structure of the ensemble.

Deprecated This function was renamed to `vrna_centroid_from_probs()`

17.10 ViennaRNA/cofold.h File Reference

MFE implementations for RNA-RNA interaction.

Include dependency graph for cofold.h:



Functions

- float [vrna_cofold](#) (const char *sequence, char *structure)
Compute Minimum Free Energy (MFE), and a corresponding secondary structure for two dimerized RNA sequences.
- float [cofold](#) (const char *sequence, char *structure)
Compute the minimum free energy of two interacting RNA molecules.
- float [cofold_par](#) (const char *string, char *structure, [vrna_param_t](#) *parameters, int is_constrained)
Compute the minimum free energy of two interacting RNA molecules.
- void [free_co_arrays](#) (void)
Free memory occupied by [cofold\(\)](#)
- void [update_cofold_params](#) (void)
Recalculate parameters.
- void [update_cofold_params_par](#) ([vrna_param_t](#) *parameters)
Recalculate parameters.
- void [export_cofold_arrays_gg](#) (int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **fc_p, int **ggg_p, int **indx_p, char **ptype_p)
Export the arrays of partition function cofold (with gquadraplex support)
- void [export_cofold_arrays](#) (int **f5_p, int **c_p, int **fML_p, int **fM1_p, int **fc_p, int **indx_p, char **ptype_p)
Export the arrays of partition function cofold.
- void [get_monomere_mfes](#) (float *e1, float *e2)
get_monomer_free_energies
- void [initialize_cofold](#) (int length)

17.10.1 Detailed Description

MFE implementations for RNA-RNA interaction.

17.11 ViennaRNA/combinatorics.h File Reference

Various implementations that deal with combinatorial aspects of RNA/DNA folding.

Functions

- unsigned int ** [vrna_enumerate_necklaces](#) (const unsigned int *type_counts)
Enumerate all necklaces with fixed content.

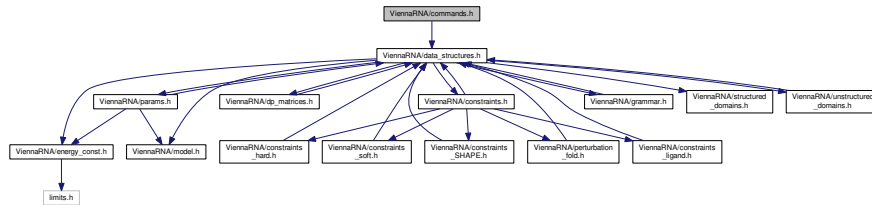
17.11.1 Detailed Description

Various implementations that deal with combinatorial aspects of RNA/DNA folding.

17.12 ViennaRNA/commands.h File Reference

Parse and apply different commands that alter the behavior of secondary structure prediction and evaluation.

Include dependency graph for commands.h:



Data Structures

- struct [vrna_command_s](#)
List element for commands ready for application to a [vrna_fold_compound_t](#).
- #define [VRNA_CMD_PARSE_HC](#) 1U
Command parse/apply flag indicating hard constraints.
- #define [VRNA_CMD_PARSE_SC](#) 2U
Command parse/apply flag indicating soft constraints.
- #define [VRNA_CMD_PARSE_UD](#) 4U
Command parse/apply flag indicating unstructured domains.
- #define [VRNA_CMD_PARSE_SD](#) 8U
Command parse/apply flag indicating structured domains.
- #define [VRNA_CMD_PARSE_DEFAULTS](#)
Command parse/apply flag indicating default set of commands.
- typedef struct [vrna_command_s](#) [vrna_cmd_t](#)
Typename for the command representing data structure [vrna_command_s](#).
- [vrna_cmd_t](#) * [vrna_file_commands_read](#) (const char *filename, unsigned int options)
Extract a list of commands from a command file.
- int [vrna_file_commands_apply](#) ([vrna_fold_compound_t](#) *vc, const char *filename, unsigned int options)
Apply a list of commands from a command file.
- int [vrna_commands_apply](#) ([vrna_fold_compound_t](#) *vc, [vrna_cmd_t](#) *commands, unsigned int options)
Apply a list of commands to a [vrna_fold_compound_t](#).
- void [vrna_commands_free](#) ([vrna_cmd_t](#) *commands)
Free memory occupied by a list of commands.

17.12.1 Detailed Description

Parse and apply different commands that alter the behavior of secondary structure prediction and evaluation.

17.12.2 Macro Definition Documentation

17.12.2.1 `#define VRNA_CMD_PARSE_HC 1U`

Command parse/apply flag indicating hard constraints.

See also

[vrna_command_s](#), [vrna_file_commands_read\(\)](#), [vrna_file_commands_apply\(\)](#), [vrna_commands_apply\(\)](#)

17.12.2.2 `#define VRNA_CMD_PARSE_SC 2U`

Command parse/apply flag indicating soft constraints.

See also

[vrna_command_s](#), [vrna_file_commands_read\(\)](#), [vrna_file_commands_apply\(\)](#), [vrna_commands_apply\(\)](#)

17.12.2.3 `#define VRNA_CMD_PARSE_UD 4U`

Command parse/apply flag indicating unstructured domains.

See also

[vrna_command_s](#), [vrna_file_commands_read\(\)](#), [vrna_file_commands_apply\(\)](#), [vrna_commands_apply\(\)](#)

17.12.2.4 `#define VRNA_CMD_PARSE_SD 8U`

Command parse/apply flag indicating structured domains.

See also

[vrna_command_s](#), [vrna_file_commands_read\(\)](#), [vrna_file_commands_apply\(\)](#), [vrna_commands_apply\(\)](#)

17.12.2.5 `#define VRNA_CMD_PARSE_DEFAULTS`

Value:

```
( VRNA_CMD_PARSE_HC \
    | VRNA_CMD_PARSE_SC \
    | VRNA_CMD_PARSE_UD \
    | VRNA_CMD_PARSE_SD \
)
```

Command parse/apply flag indicating default set of commands.

See also

[vrna_command_s](#), [vrna_file_commands_read\(\)](#), [vrna_file_commands_apply\(\)](#), [vrna_commands_apply\(\)](#)

17.12.3 Function Documentation

17.12.3.1 `vrna_cmd_t* vrna_file_commands_read (const char * filename, unsigned int options)`

Extract a list of commands from a command file.

Read a list of commands specified in the input file and return them as list of abstract commands

See also

[vrna_commands_apply\(\)](#), [vrna_file_commands_apply\(\)](#), [vrna_commands_free\(\)](#)

Parameters

<i>filename</i>	The filename
<i>options</i>	Options to limit the type of commands read from the file

Returns

A list of abstract commands

17.12.3.2 `int vrna_file_commands_apply (vrna_fold_compound_t * vc, const char * filename, unsigned int options)`

Apply a list of commands from a command file.

This function is a shortcut to directly parse a commands file and apply all successfully parsed commands to a [vrna_fold_compound_t](#) data structure. It is the same as:

```
int          r;
vrna_cmd_t  *cmds;

cmds = vrna_file_commands_read(filename, options);
r    = vrna_commands_apply(vc, cmds, options);

vrna_commands_free(cmds);

return r;
```

Parameters

<i>vc</i>	The vrna_fold_compound_t the command list will be applied to
<i>filename</i>	The filename
<i>options</i>	Options to limit the type of commands read from the file

Returns

The number of commands successfully applied

SWIG Wrapper Notes This function is attached as method `file_commands_apply()` to objects of type `fold_↔
compound`

17.12.3.3 `int vrna_commands_apply (vrna_fold_compound_t * vc, vrna_cmd_t * commands, unsigned int options)`

Apply a list of commands to a [vrna_fold_compound_t](#).

Parameters

<i>vc</i>	The vrna_fold_compound_t the command list will be applied to
<i>commands</i>	The list of commands to apply
<i>options</i>	Options to limit the type of commands read from the file

Returns

The number of commands successfully applied

SWIG Wrapper Notes This function is attached as method **commands_apply()** to objects of type *fold_compound*

17.12.3.4 void vrna_commands_free (vrna_cmd_t * commands)

Free memory occupied by a list of commands.

Release memory occupied by a list of commands

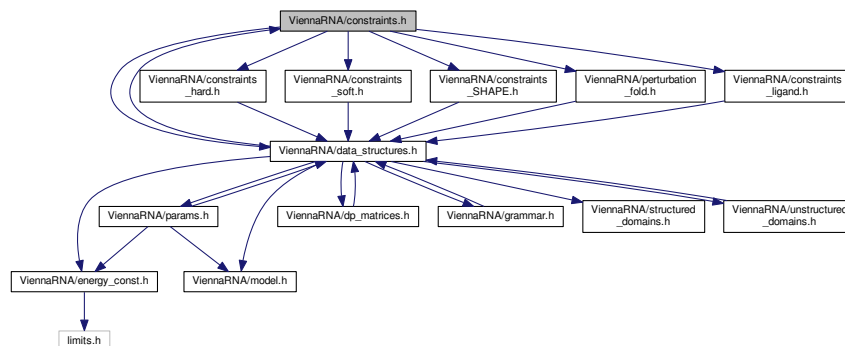
Parameters

<i>commands</i>	A pointer to a list of commands
-----------------	---------------------------------

17.13 ViennaRNA/constraints.h File Reference

Functions and data structures for constraining secondary structure predictions and evaluation.

Include dependency graph for constraints.h:



This graph shows which files directly or indirectly include this file:



Macros

- **#define VRNA_CONSTRAINT_FILE 0**
Flag for *vrna_constraints_add()* to indicate that constraints are present in a text file.
- **#define VRNA_CONSTRAINT_SOFT_MFE 0**

- Indicate generation of constraints for MFE folding.*

 - `#define VRNA_CONSTRAINT_SOFT_PF VRNA_OPTION_PF`

Indicate generation of constraints for partition function computation.
- `#define VRNA_DECOMP_PAIR_HP 1`

Flag passed to generic softt constraints callback to indicate hairpin loop decomposition step.
- `#define VRNA_DECOMP_PAIR_IL 2`

Indicator for interior loop decomposition step.
- `#define VRNA_DECOMP_PAIR_ML 3`

Indicator for multibranch loop decomposition step.
- `#define VRNA_DECOMP_ML_ML_ML 5`

Indicator for decomposition of multibranch loop part.
- `#define VRNA_DECOMP_ML_STEM 4`

Indicator for decomposition of multibranch loop part.
- `#define VRNA_DECOMP_ML_ML 6`

Indicator for decomposition of multibranch loop part.
- `#define VRNA_DECOMP_ML_UP 11`

Indicator for decomposition of multibranch loop part.
- `#define VRNA_DECOMP_ML_ML_STEM 20`

Indicator for decomposition of multibranch loop part.
- `#define VRNA_DECOMP_ML_COAXIAL 13`

Indicator for decomposition of multibranch loop part.
- `#define VRNA_DECOMP_EXT_EXT 9`

Indicator for decomposition of exterior loop part.
- `#define VRNA_DECOMP_EXT_UP 8`

Indicator for decomposition of exterior loop part.
- `#define VRNA_DECOMP_EXT_STEM 14`

Indicator for decomposition of exterior loop part.
- `#define VRNA_DECOMP_EXT_EXT_EXT 15`

Indicator for decomposition of exterior loop part.
- `#define VRNA_DECOMP_EXT_STEM_EXT 16`

Indicator for decomposition of exterior loop part.
- `#define VRNA_DECOMP_EXT_STEM_OUTSIDE 17`

Indicator for decomposition of exterior loop part.
- `#define VRNA_DECOMP_EXT_EXT_STEM 18`

Indicator for decomposition of exterior loop part.
- `#define VRNA_DECOMP_EXT_EXT_STEM1 19`

Indicator for decomposition of exterior loop part.

Functions

- `void vrna_constraints_add (vrna_fold_compound_t *vc, const char *constraint, unsigned int options)`

Add constraints to a `vrna_fold_compound_t` data structure.

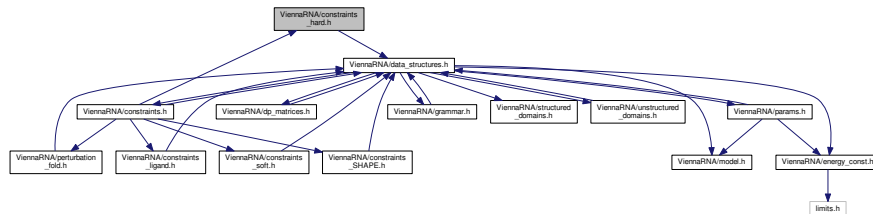
17.13.1 Detailed Description

Functions and data structures for constraining secondary structure predictions and evaluation.

17.14 ViennaRNA/constraints_hard.h File Reference

Functions and data structures for handling of secondary structure hard constraints.

Include dependency graph for constraints_hard.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [vrna_hc_s](#)
The hard constraints data structure. [More...](#)
- struct [vrna_hc_up_s](#)
A single hard constraint for a single nucleotide. [More...](#)

Macros

- `#define VRNA_CONSTRAINT_NO_HEADER 0`
do not print the header information line
- `#define VRNA_CONSTRAINT_DB 16384U`
Flag for [vrna_constraints_add\(\)](#) to indicate that constraint is passed in pseudo dot-bracket notation.
- `#define VRNA_CONSTRAINT_DB_ENFORCE_BP 32768U`
Switch for dot-bracket structure constraint to enforce base pairs.
- `#define VRNA_CONSTRAINT_DB_PIPE 65536U`
Flag that is used to indicate the pipe '|' sign in pseudo dot-bracket notation of hard constraints.
- `#define VRNA_CONSTRAINT_DB_DOT 131072U`
dot '.' switch for structure constraints (no constraint at all)
- `#define VRNA_CONSTRAINT_DB_X 262144U`
'x' switch for structure constraint (base must not pair)
- `#define VRNA_CONSTRAINT_DB_ANG_BRACK 524288U`
angle brackets '<', '>' switch for structure constraint (paired downstream/upstream)
- `#define VRNA_CONSTRAINT_DB_RND_BRACK 1048576U`
round brackets '(', ')' switch for structure constraint (base i pairs base j)
- `#define VRNA_CONSTRAINT_DB_INTRAMOL 2097152U`
Flag that is used to indicate the character 'I' in pseudo dot-bracket notation of hard constraints.

- `#define VRNA_CONSTRAINT_DB_INTERMOL 4194304U`
Flag that is used to indicate the character 'e' in pseudo dot-bracket notation of hard constraints.
- `#define VRNA_CONSTRAINT_DB_GQUAD 8388608U`
'+' switch for structure constraint (base is involved in a gquad)
- `#define VRNA_CONSTRAINT_DB_DEFAULT`
Switch for dot-bracket structure constraint with default symbols.
- `#define VRNA_CONSTRAINT_CONTEXT_EXT_LOOP (char)0x01`
Hard constraints flag, base pair in the exterior loop.
- `#define VRNA_CONSTRAINT_CONTEXT_HP_LOOP (char)0x02`
Hard constraints flag, base pair encloses hairpin loop.
- `#define VRNA_CONSTRAINT_CONTEXT_INT_LOOP (char)0x04`
Hard constraints flag, base pair encloses an interior loop.
- `#define VRNA_CONSTRAINT_CONTEXT_INT_LOOP_ENC (char)0x08`
Hard constraints flag, base pair encloses a multi branch loop.
- `#define VRNA_CONSTRAINT_CONTEXT_MB_LOOP (char)0x10`
Hard constraints flag, base pair is enclosed in an interior loop.
- `#define VRNA_CONSTRAINT_CONTEXT_MB_LOOP_ENC (char)0x20`
Hard constraints flag, base pair is enclosed in a multi branch loop.
- `#define VRNA_CONSTRAINT_CONTEXT_ENFORCE (char)0x40`
Hard constraint flag to indicate enforcement of constraints.
- `#define VRNA_CONSTRAINT_CONTEXT_NO_REMOVE (char)0x80`
Hard constraint flag to indicate not to remove base pairs that conflict with a given constraint.
- `#define VRNA_CONSTRAINT_CONTEXT_ALL_LOOPS`
Hard constraints flag, shortcut for all base pairs.

Typedefs

- `typedef struct vrna_hc_s vrna_hc_t`
Typename for the hard constraints data structure `vrna_hc_s`.
- `typedef struct vrna_hc_up_s vrna_hc_up_t`
Typename for the single nucleotide hard constraint data structure `vrna_hc_up_s`.
- `typedef char(vrna_callback_hc_evaluate)(int i, int j, int k, int l, char d, void *data)`
Callback to evaluate whether or not a particular decomposition step is contributing to the solution space.

Functions

- `void vrna_message_constraint_options(unsigned int option)`
Print a help message for pseudo dot-bracket structure constraint characters to stdout. (constraint support is specified by option parameter)
- `void vrna_message_constraint_options_all(void)`
Print structure constraint characters to stdout (full constraint support)
- `void vrna_hc_init(vrna_fold_compound_t *vc)`
Initialize/Reset hard constraints to default values.
- `void vrna_hc_add_up(vrna_fold_compound_t *vc, int i, char option)`
Make a certain nucleotide unpaired.
- `int vrna_hc_add_up_batch(vrna_fold_compound_t *vc, vrna_hc_up_t *constraints)`
Apply a list of hard constraints for single nucleotides.
- `void vrna_hc_add_bp(vrna_fold_compound_t *vc, int i, int j, char option)`
Favorize/Enforce a certain base pair (i,j)

- void [vrna_hc_add_bp_nonspecific](#) ([vrna_fold_compound_t](#) *vc, int i, int d, char option)
Enforce a nucleotide to be paired (upstream/downstream)
- void [vrna_hc_free](#) ([vrna_hc_t](#) *hc)
Free the memory allocated by a [vrna_hc_t](#) data structure.
- int [vrna_hc_add_from_db](#) ([vrna_fold_compound_t](#) *vc, const char *constraint, unsigned int options)
Add hard constraints from pseudo dot-bracket notation.
- void [print_tty_constraint](#) (unsigned int option)
Print structure constraint characters to stdout. (constraint support is specified by option parameter)
- void [print_tty_constraint_full](#) (void)
Print structure constraint characters to stdout (full constraint support)
- void [constrain_ptypes](#) (const char *constraint, unsigned int length, char *ptype, int *BP, int min_loop_size, unsigned int idx_type)
Insert constraining pair types according to constraint structure string.

17.14.1 Detailed Description

Functions and data structures for handling of secondary structure hard constraints.

17.14.2 Macro Definition Documentation

17.14.2.1 `#define VRNA_CONSTRAINT_NO_HEADER 0`

do not print the header information line

Deprecated This mode is not supported anymore!

17.14.2.2 `#define VRNA_CONSTRAINT_DB_ANG_BRACK 524288U`

angle brackets '<', '>' switch for structure constraint (paired downstream/upstream)

See also

[vrna_hc_add_from_db\(\)](#), [vrna_constraints_add\(\)](#), [vrna_message_constraint_options\(\)](#), [vrna_message_constraint_options_all\(\)](#)

17.14.3 Function Documentation

17.14.3.1 void [print_tty_constraint](#) (unsigned int *option*)

Print structure constraint characters to stdout. (constraint support is specified by option parameter)

Deprecated Use [vrna_message_constraints\(\)](#) instead!

Parameters

<i>option</i>	Option switch that tells which constraint help will be printed
---------------	----------------------------------------------------------------

17.14.3.2 void print_tty_constraint_full (void)

Print structure constraint characters to stdout (full constraint support)

Deprecated Use [vrna_message_constraint_options_all\(\)](#) instead!

17.14.3.3 void constrain_ptypes (const char * *constraint*, unsigned int *length*, char * *ptype*, int * *BP*, int *min_loop_size*, unsigned int *idx_type*)

Insert constraining pair types according to constraint structure string.

Deprecated Do not use this function anymore! Structure constraints are now handled through [vrna_hc_t](#) and related functions.

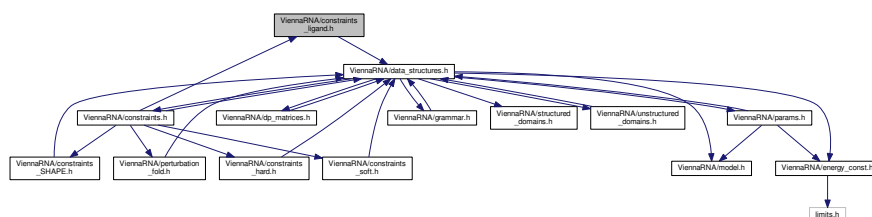
Parameters

<i>constraint</i>	The structure constraint string
<i>length</i>	The actual length of the sequence (constraint may be shorter)
<i>ptype</i>	A pointer to the basepair type array
<i>BP</i>	(not used anymore)
<i>min_loop_size</i>	The minimal loop size (usually TURN)
<i>idx_type</i>	Define the access type for base pair type array (0 = indx, 1 = iindx)

17.15 ViennaRNA/constraints_ligand.h File Reference

Functions for incorporation of ligands binding to hairpin and interior loop motifs using the soft constraints framework.

Include dependency graph for constraints_ligand.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [vrna_sc_motif_s](#)

Functions

- int [vrna_sc_add_hi_motif](#) ([vrna_fold_compound_t](#) *vc, const char *seq, const char *structure, [FLT_OR_DBL](#) energy, unsigned int options)

Add soft constraints for hairpin or interior loop binding motif.

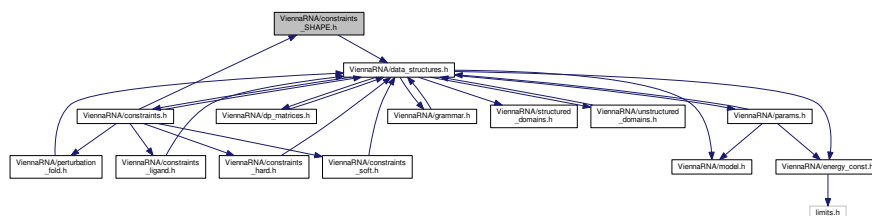
17.15.1 Detailed Description

Functions for incorporation of ligands binding to hairpin and interior loop motifs using the soft constraints framework.

17.16 ViennaRNA/constraints_SHAPE.h File Reference

This module provides function to incorporate SHAPE reactivity data into the folding recursions by means of soft constraints.

Include dependency graph for constraints_SHAPE.h:



This graph shows which files directly or indirectly include this file:



Functions

- int [vrna_sc_add_SHAPE_deigan](#) ([vrna_fold_compound_t](#) *vc, const double *reactivities, double m, double b, unsigned int options)
Add SHAPE reactivity data as soft constraints (Deigan et al. method)
- int [vrna_sc_add_SHAPE_deigan_al](#)i ([vrna_fold_compound_t](#) *vc, const char **shape_files, const int *shape_file_association, double m, double b, unsigned int options)
Add SHAPE reactivity data from files as soft constraints for consensus structure prediction (Deigan et al. method)
- int [vrna_sc_add_SHAPE_zarringhalam](#) ([vrna_fold_compound_t](#) *vc, const double *reactivities, double b, double default_value, const char *shape_conversion, unsigned int options)
Add SHAPE reactivity data as soft constraints (Zarringhalam et al. method)
- int [vrna_sc_SHAPE_parse_method](#) (const char *method_string, char *method, float *param_1, float *param_2)
Parse a character string and extract the encoded SHAPE reactivity conversion method and possibly the parameters for conversion into pseudo free energies.
- int [vrna_sc_SHAPE_to_pr](#) (const char *shape_conversion, double *values, int length, double default_value)
Convert SHAPE reactivity values to probabilities for being unpaired.

17.16.1 Detailed Description

This module provides function to incorporate SHAPE reactivity data into the folding recursions by means of soft constraints.

17.16.2 Function Documentation

17.16.2.1 int vrna_sc_SHAPE_parse_method (const char * method_string, char * method, float * param_1, float * param_2)

Parse a character string and extract the encoded SHAPE reactivity conversion method and possibly the parameters for conversion into pseudo free energies.

Parameters

<i>method_string</i>	The string that contains the encoded SHAPE reactivity conversion method
<i>method</i>	A pointer to the memory location where the method character will be stored
<i>param_1</i>	A pointer to the memory location where the first parameter of the corresponding method will be stored
<i>param_2</i>	A pointer to the memory location where the second parameter of the corresponding method will be stored

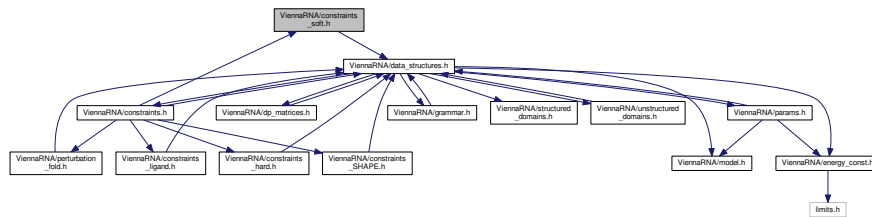
Returns

1 on successful extraction of the method, 0 on errors

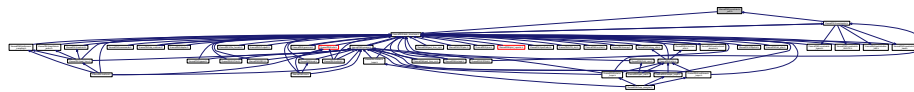
17.17 ViennaRNA/constraints_soft.h File Reference

Functions and data structures for secondary structure soft constraints.

Include dependency graph for constraints_soft.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [vrna_sc_s](#)
The soft constraints data structure. [More...](#)

Typedefs

- typedef struct [vrna_sc_s](#) [vrna_sc_t](#)
Typename for the soft constraints data structure [vrna_sc_s](#).
- typedef int([vrna_callback_sc_energy](#)) (int i, int j, int k, int l, char d, void *data)
Callback to retrieve pseudo energy contribution for soft constraint feature.
- typedef FLT_OR_DBL([vrna_callback_sc_exp_energy](#)) (int i, int j, int k, int l, char d, void *data)
Callback to retrieve pseudo energy contribution as Boltzmann Factors for soft constraint feature.
- typedef [vrna_basepair_t](#) *([vrna_callback_sc_backtrack](#)) (int i, int j, int k, int l, char d, void *data)
Callback to retrieve auxiliary base pairs for soft constraint feature.

Functions

- void [vrna_sc_init](#) ([vrna_fold_compound_t](#) *vc)
Initialize an empty soft constraints data structure within a [vrna_fold_compound_t](#).
- void [vrna_sc_set_bp](#) ([vrna_fold_compound_t](#) *vc, const FLT_OR_DBL **constraints, unsigned int options)
Set soft constraints for paired nucleotides.
- void [vrna_sc_add_bp](#) ([vrna_fold_compound_t](#) *vc, int i, int j, FLT_OR_DBL energy, unsigned int options)
Add soft constraints for paired nucleotides.
- void [vrna_sc_set_up](#) ([vrna_fold_compound_t](#) *vc, const FLT_OR_DBL *constraints, unsigned int options)
Set soft constraints for unpaired nucleotides.
- void [vrna_sc_add_up](#) ([vrna_fold_compound_t](#) *vc, int i, FLT_OR_DBL energy, unsigned int options)
Add soft constraints for unpaired nucleotides.
- void [vrna_sc_remove](#) ([vrna_fold_compound_t](#) *vc)
Remove soft constraints from [vrna_fold_compound_t](#).

- void [vrna_sc_free](#) ([vrna_sc_t](#) *sc)
Free memory occupied by a [vrna_sc_t](#) data structure.
- void [vrna_sc_add_data](#) ([vrna_fold_compound_t](#) *vc, void *data, [vrna_callback_free_auxdata](#) *free_data)
Add an auxiliary data structure for the generic soft constraints callback function.
- void [vrna_sc_add_f](#) ([vrna_fold_compound_t](#) *vc, [vrna_callback_sc_energy](#) *f)
Bind a function pointer for generic soft constraint feature (MFE version)
- void [vrna_sc_add_bt](#) ([vrna_fold_compound_t](#) *vc, [vrna_callback_sc_backtrack](#) *f)
Bind a backtracking function pointer for generic soft constraint feature.
- void [vrna_sc_add_exp_f](#) ([vrna_fold_compound_t](#) *vc, [vrna_callback_sc_exp_energy](#) *exp_f)
Bind a function pointer for generic soft constraint feature (PF version)

17.17.1 Detailed Description

Functions and data structures for secondary structure soft constraints.

17.18 ViennaRNA/convert_epars.h File Reference

Functions and definitions for energy parameter file format conversion.

Macros

- #define [VRNA_CONVERT_OUTPUT_ALL](#) 1U
- #define [VRNA_CONVERT_OUTPUT_HP](#) 2U
- #define [VRNA_CONVERT_OUTPUT_STACK](#) 4U
- #define [VRNA_CONVERT_OUTPUT_MM_HP](#) 8U
- #define [VRNA_CONVERT_OUTPUT_MM_INT](#) 16U
- #define [VRNA_CONVERT_OUTPUT_MM_INT_1N](#) 32U
- #define [VRNA_CONVERT_OUTPUT_MM_INT_23](#) 64U
- #define [VRNA_CONVERT_OUTPUT_MM_MULTI](#) 128U
- #define [VRNA_CONVERT_OUTPUT_MM_EXT](#) 256U
- #define [VRNA_CONVERT_OUTPUT_DANGLE5](#) 512U
- #define [VRNA_CONVERT_OUTPUT_DANGLE3](#) 1024U
- #define [VRNA_CONVERT_OUTPUT_INT_11](#) 2048U
- #define [VRNA_CONVERT_OUTPUT_INT_21](#) 4096U
- #define [VRNA_CONVERT_OUTPUT_INT_22](#) 8192U
- #define [VRNA_CONVERT_OUTPUT_BULGE](#) 16384U
- #define [VRNA_CONVERT_OUTPUT_INT](#) 32768U
- #define [VRNA_CONVERT_OUTPUT_ML](#) 65536U
- #define [VRNA_CONVERT_OUTPUT_MISC](#) 131072U
- #define [VRNA_CONVERT_OUTPUT_SPECIAL_HP](#) 262144U
- #define [VRNA_CONVERT_OUTPUT_VANILLA](#) 524288U
- #define [VRNA_CONVERT_OUTPUT_NINIO](#) 1048576U
- #define [VRNA_CONVERT_OUTPUT_DUMP](#) 2097152U

Functions

- void [convert_parameter_file](#) (const char *iname, const char *oname, unsigned int options)

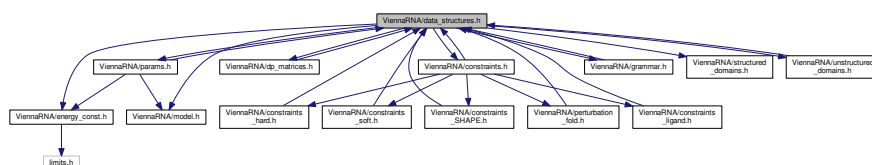
17.18.1 Detailed Description

Functions and definitions for energy parameter file format conversion.

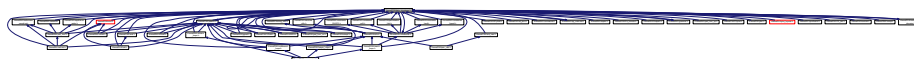
17.19 ViennaRNA/data_structures.h File Reference

Various data structures and pre-processor macros.

Include dependency graph for data_structures.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [vrna_basepair_s](#)
Base pair data structure used in subopt.c. [More...](#)
- struct [vrna_plist_s](#)
this datastructure is used as input parameter in functions of [PS_dot.h](#) and others [More...](#)
- struct [vrna_cpair_s](#)
this datastructure is used as input parameter in functions of [PS_dot.c](#) [More...](#)
- struct [vrna_color_s](#)
- struct [vrna_data_linear_s](#)
- struct [vrna_sect_s](#)
Stack of partial structures for backtracking. [More...](#)
- struct [vrna_bp_stack_s](#)
Base pair stack element. [More...](#)
- struct [pu_contrib](#)
contributions to p_u [More...](#)
- struct [interact](#)
interaction data structure for RNAup [More...](#)
- struct [pu_out](#)
Collection of all free_energy of beeing unpaired values for output. [More...](#)
- struct [constrain](#)
constraints for cofolding [More...](#)
- struct [duplexT](#)
Data structure for RNAduplex. [More...](#)
- struct [node](#)

- *Data structure for RNAsnoop (fold energy list)* [More...](#)
- struct [snoopT](#)
Data structure for RNAsnoop. [More...](#)
- struct [dupVar](#)
Data structure used in RNApkplex. [More...](#)
- struct [vrna_fc_s](#)
The most basic data structure required by many functions throughout the RNAlib. [More...](#)

Macros

- #define [VRNA_STATUS_MFE_PRE](#) (unsigned char)1
Status message indicating that MFE computations are about to begin.
- #define [VRNA_STATUS_MFE_POST](#) (unsigned char)2
Status message indicating that MFE computations are finished.
- #define [VRNA_STATUS_PF_PRE](#) (unsigned char)3
Status message indicating that Partition function computations are about to begin.
- #define [VRNA_STATUS_PF_POST](#) (unsigned char)4
Status message indicating that Partition function computations are finished.
- #define [VRNA_OPTION_DEFAULT](#) 0U
Option flag to specify default settings/requirements.
- #define [VRNA_OPTION_MFE](#) 1U
Option flag to specify requirement of Minimum Free Energy (MFE) DP matrices and corresponding set of energy parameters.
- #define [VRNA_OPTION_PF](#) 2U
Option flag to specify requirement of Partition Function (PF) DP matrices and corresponding set of Boltzmann factors.
- #define [VRNA_OPTION_HYBRID](#) 4U
Option flag to specify requirement of dimer DP matrices.
- #define [VRNA_OPTION_EVAL_ONLY](#) 8U
Option flag to specify that neither MFE, nor PF DP matrices are required.
- #define [VRNA_OPTION_WINDOW](#) 16U
Option flag to specify requirement of DP matrices for local folding approaches.

Typedefs

- typedef struct [vrna_fc_s](#) [vrna_fold_compound_t](#)
Typename for the fold_compound data structure [vrna_fc_s](#).
- typedef struct [vrna_basepair_s](#) [vrna_basepair_t](#)
Typename for the base pair representing data structure [vrna_basepair_s](#).
- typedef struct [vrna_plist_s](#) [vrna_plist_t](#)
Typename for the base pair list representing data structure [vrna_plist_s](#).
- typedef struct [vrna_bp_stack_s](#) [vrna_bp_stack_t](#)
Typename for the base pair stack representing data structure [vrna_bp_stack_s](#).
- typedef struct [vrna_cpair_s](#) [vrna_cpair_t](#)
Typename for data structure [vrna_cpair_s](#).
- typedef struct [vrna_sect_s](#) [vrna_sect_t](#)
Typename for stack of partial structures [vrna_sect_s](#).
- typedef double [FLT_OR_DBL](#)
Typename for floating point number in partition function computations.
- typedef void([vrna_callback_free_auxdata](#)) (void *data)

- *Callback to free memory allocated for auxiliary user-provided data.*
- typedef void([vrna_callback_recursion_status](#)) (unsigned char status, void *data)
Callback to perform specific user-defined actions before, or after recursive computations.
- typedef struct [vrna_basepair_s](#) PAIR
Old typename of [vrna_basepair_s](#).
- typedef struct [vrna_plist_s](#) plist
Old typename of [vrna_plist_s](#).
- typedef struct [vrna_cpair_s](#) cpair
Old typename of [vrna_cpair_s](#).
- typedef struct [vrna_sect_s](#) sect
Old typename of [vrna_sect_s](#).
- typedef struct [vrna_bp_stack_s](#) bondT
Old typename of [vrna_bp_stack_s](#).
- typedef struct [pu_contrib](#) pu_contrib
contributions to p_u
- typedef struct [interact](#) interact
interaction data structure for RNAup
- typedef struct [pu_out](#) pu_out
Collection of all free_energy of beeing unpaired values for output.
- typedef struct [constrain](#) constrain
constraints for cofolding
- typedef struct [node](#) folden
Data structure for RNAsnoop (fold energy list)
- typedef struct [dupVar](#) dupVar
Data structure used in RNApkplex.

Enumerations

Functions

- void [vrna_C11_features](#) (void)
Dummy symbol to check whether the library was build using C11/C++11 features.
- [vrna_fold_compound_t](#) * [vrna_fold_compound](#) (const char *sequence, [vrna_md_t](#) *md_p, unsigned int options)
Retrieve a [vrna_fold_compound_t](#) data structure for single sequences and hybridizing sequences.
- [vrna_fold_compound_t](#) * [vrna_fold_compound_comparative](#) (const char **sequences, [vrna_md_t](#) *md_p, unsigned int options)
Retrieve a [vrna_fold_compound_t](#) data structure for sequence alignments.
- void [vrna_fold_compound_free](#) ([vrna_fold_compound_t](#) *vc)
Free memory occupied by a [vrna_fold_compound_t](#).
- void [vrna_fold_compound_add_auxdata](#) ([vrna_fold_compound_t](#) *vc, void *data, [vrna_callback_free_](#)↵
[auxdata](#) *f)
Add auxiliary data to the [vrna_fold_compound_t](#).
- void [vrna_fold_compound_add_callback](#) ([vrna_fold_compound_t](#) *vc, [vrna_callback_recursion_status](#) *f)
Add a recursion status callback to the [vrna_fold_compound_t](#).

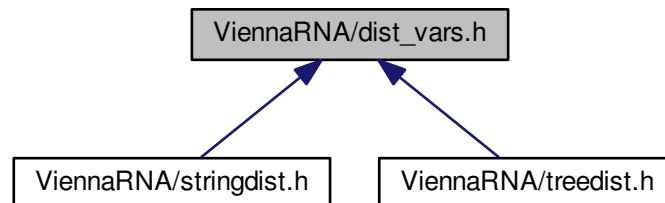
17.19.1 Detailed Description

Various data structures and pre-processor macros.

17.20 ViennaRNA/dist_vars.h File Reference

Global variables for Distance-Package.

This graph shows which files directly or indirectly include this file:



Data Structures

- struct [Postorder_list](#)
Postorder data structure.
- struct [Tree](#)
Tree data structure.
- struct [swString](#)
Some other data structure.

Variables

- int [edit_backtrack](#)
Produce an alignment of the two structures being compared by tracing the editing path giving the minimum distance.
- char * [aligned_line](#) [4]
Contains the two aligned structures after a call to one of the distance functions with [edit_backtrack](#) set to 1.
- int [cost_matrix](#)
Specify the cost matrix to be used for distance calculations.

17.20.1 Detailed Description

Global variables for Distance-Package.

17.20.2 Variable Documentation

17.20.2.1 int edit_backtrack

Produce an alignment of the two structures being compared by tracing the editing path giving the minimum distance.
set to 1 if you want backtracking

Enumerations

Functions

- int `vrna_mx_add` (`vrna_fold_compound_t` *vc, `vrna_mx_type_e` type, unsigned int options)
Add Dynamic Programming (DP) matrices (allocate memory)
- void `vrna_mx_mfe_free` (`vrna_fold_compound_t` *vc)
Free memory occupied by the Minimum Free Energy (MFE) Dynamic Programming (DP) matrices.
- void `vrna_mx_pf_free` (`vrna_fold_compound_t` *vc)
Free memory occupied by the Partition Function (PF) Dynamic Programming (DP) matrices.

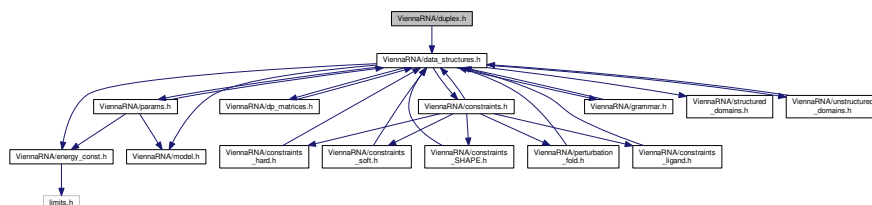
17.21.1 Detailed Description

Functions to deal with standard dynamic programming (DP) matrices.

17.22 ViennaRNA/duplex.h File Reference

Functions for simple RNA-RNA duplex interactions.

Include dependency graph for duplex.h:



17.22.1 Detailed Description

Functions for simple RNA-RNA duplex interactions.

17.23 ViennaRNA/edit_cost.h File Reference

global variables for Edit Costs included by treedist.c and stringdist.c

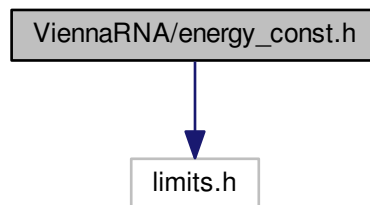
17.23.1 Detailed Description

global variables for Edit Costs included by treedist.c and stringdist.c

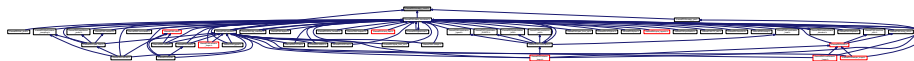
17.24 ViennaRNA/energy_const.h File Reference

Energy parameter constants.

Include dependency graph for energy_const.h:



This graph shows which files directly or indirectly include this file:



Macros

- `#define GASCONST 1.98717 /* in [cal/K] */`
- `#define K0 273.15`
- `#define INF 10000000 /* (INT_MAX/10) */`
- `#define FORBIDDEN 9999`
- `#define BONUS 10000`
- `#define NBPAIRS 7`
- `#define TURN 3`
- `#define MAXLOOP 30`

17.24.1 Detailed Description

Energy parameter constants.

17.24.2 Macro Definition Documentation

17.24.2.1 `#define GASCONST 1.98717 /* in [cal/K] */`

The gas constant

17.24.2.2 `#define K0 273.15`

0 deg Celsius in Kelvin

17.24.2.3 `#define INF 10000000 /* (INT_MAX/10) */`

Infinity as used in minimization routines

17.24.2.4 `#define FORBIDDEN 9999`

forbidden

17.24.2.5 `#define BONUS 10000`

bonus contribution

17.24.2.6 `#define NBPAIRS 7`

The number of distinguishable base pairs

17.24.2.7 `#define TURN 3`

The minimum loop length

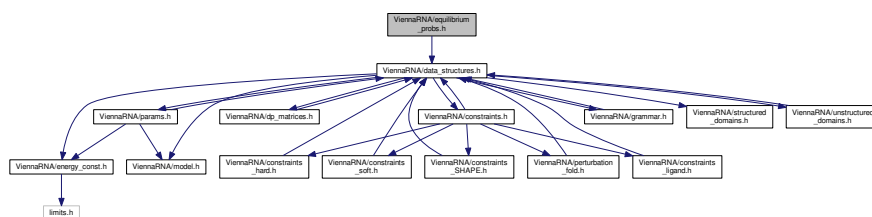
17.24.2.8 `#define MAXLOOP 30`

The maximum loop length

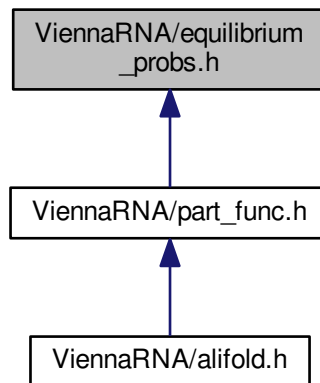
17.25 ViennaRNA/equilibrium_probs.h File Reference

Equilibrium Probability implementations.

Include dependency graph for equilibrium_probs.h:



This graph shows which files directly or indirectly include this file:



Functions

- double [vrna_mean_bp_distance_pr](#) (int length, [FLT_OR_DBL](#) *pr)
Get the mean base pair distance in the thermodynamic ensemble from a probability matrix.
- double [vrna_mean_bp_distance](#) ([vrna_fold_compound_t](#) *vc)
Get the mean base pair distance in the thermodynamic ensemble.
- [vrna_plist_t](#) * [vrna_stack_prob](#) ([vrna_fold_compound_t](#) *vc, double cutoff)
Compute stacking probabilities.

17.25.1 Detailed Description

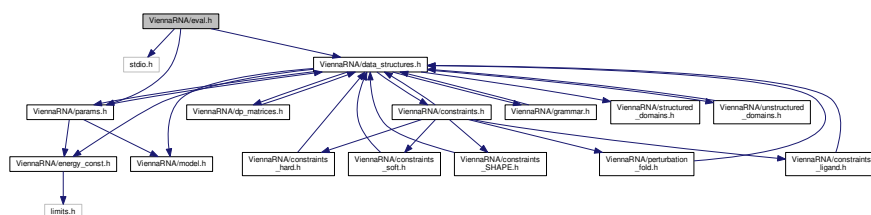
Equilibrium Probability implementations.

This file includes various implementations for equilibrium probability computations based on the partition function of an RNA sequence, two concatenated sequences, or a sequence alignment.

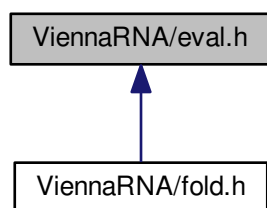
17.26 ViennaRNA/eval.h File Reference

Functions and variables related to energy evaluation of sequence/structure pairs.

Include dependency graph for eval.h:



This graph shows which files directly or indirectly include this file:



Functions

- float [vrna_eval_structure](#) ([vrna_fold_compound_t](#) *vc, const char *structure)
Calculate the free energy of an already folded RNA.
- float [vrna_eval_covar_structure](#) ([vrna_fold_compound_t](#) *vc, const char *structure)
Calculate the pseudo energy derived by the covariance scores of a set of aligned sequences.
- float [vrna_eval_structure_simple](#) (const char *string, const char *structure)
Calculate the free energy of an already folded RNA.
- float [vrna_eval_structure_verbose](#) ([vrna_fold_compound_t](#) *vc, const char *structure, FILE *file)
Calculate the free energy of an already folded RNA and print contributions on a per-loop base.
- float [vrna_eval_structure_v](#) ([vrna_fold_compound_t](#) *vc, const char *structure, int verbosity_level, FILE *file)
Calculate the free energy of an already folded RNA and print contributions on a per-loop base.
- float [vrna_eval_structure_simple_verbose](#) (const char *string, const char *structure, FILE *file)
Calculate the free energy of an already folded RNA and print contributions per loop.
- float [vrna_eval_structure_simple_v](#) (const char *string, const char *structure, int verbosity_level, FILE *file)
Calculate the free energy of an already folded RNA and print contributions per loop.
- int [vrna_eval_structure_pt](#) ([vrna_fold_compound_t](#) *vc, const short *pt)
Calculate the free energy of an already folded RNA.
- int [vrna_eval_structure_pt_simple](#) (const char *string, const short *pt)
Calculate the free energy of an already folded RNA.
- int [vrna_eval_structure_pt_verbose](#) ([vrna_fold_compound_t](#) *vc, const short *pt, FILE *file)
Calculate the free energy of an already folded RNA.
- int [vrna_eval_structure_pt_v](#) ([vrna_fold_compound_t](#) *vc, const short *pt, int verbosity_level, FILE *file)
Calculate the free energy of an already folded RNA.
- int [vrna_eval_structure_pt_simple_verbose](#) (const char *string, const short *pt, FILE *file)
Calculate the free energy of an already folded RNA.
- int [vrna_eval_structure_pt_simple_v](#) (const char *string, const short *pt, int verbosity_level, FILE *file)
Calculate the free energy of an already folded RNA.
- int [vrna_eval_loop_pt](#) ([vrna_fold_compound_t](#) *vc, int i, const short *pt)
Calculate energy of a loop.
- float [vrna_eval_move](#) ([vrna_fold_compound_t](#) *vc, const char *structure, int m1, int m2)
Calculate energy of a move (closing or opening of a base pair)
- int [vrna_eval_move_pt](#) ([vrna_fold_compound_t](#) *vc, short *pt, int m1, int m2)
Calculate energy of a move (closing or opening of a base pair)
- float [energy_of_structure](#) (const char *string, const char *structure, int verbosity_level)

Calculate the free energy of an already folded RNA using global model detail settings.

- float [energy_of_struct_par](#) (const char *string, const char *structure, [vrna_param_t](#) *parameters, int verbosity_level)

Calculate the free energy of an already folded RNA.

- float [energy_of_circ_structure](#) (const char *string, const char *structure, int verbosity_level)

Calculate the free energy of an already folded circular RNA.

- float [energy_of_circ_struct_par](#) (const char *string, const char *structure, [vrna_param_t](#) *parameters, int verbosity_level)

Calculate the free energy of an already folded circular RNA.

- int [energy_of_structure_pt](#) (const char *string, short *ptable, short *s, short *s1, int verbosity_level)

Calculate the free energy of an already folded RNA.

- int [energy_of_struct_pt_par](#) (const char *string, short *ptable, short *s, short *s1, [vrna_param_t](#) *parameters, int verbosity_level)

Calculate the free energy of an already folded RNA.

- float [energy_of_move](#) (const char *string, const char *structure, int m1, int m2)

Calculate energy of a move (closing or opening of a base pair)

- int [energy_of_move_pt](#) (short *pt, short *s, short *s1, int m1, int m2)

Calculate energy of a move (closing or opening of a base pair)

- int [loop_energy](#) (short *ptable, short *s, short *s1, int i)

Calculate energy of a loop.

- float [energy_of_struct](#) (const char *string, const char *structure)
- int [energy_of_struct_pt](#) (const char *string, short *ptable, short *s, short *s1)
- float [energy_of_circ_struct](#) (const char *string, const char *structure)

Variables

- int [cut_point](#)
set to first pos of second seq for cofolding
- int [eos_debug](#)
verbose info from energy_of_struct

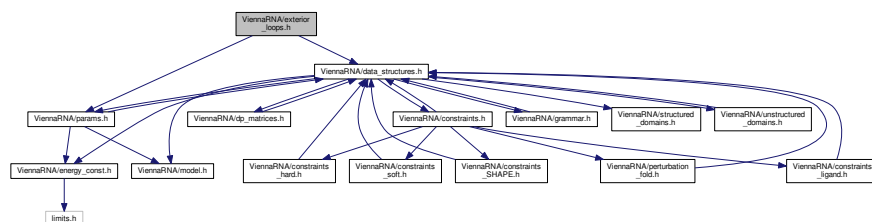
17.26.1 Detailed Description

Functions and variables related to energy evaluation of sequence/structure pairs.

17.27 ViennaRNA/exterior_loops.h File Reference

Energy evaluation of exterior loops for MFE and partition function calculations.

Include dependency graph for exterior_loops.h:



```
graph BT; A[ViennaRNA/loop_energies.h] --> B[ViennaRNA/exterior_loops.h];
```

- `int E_ExtLoop` (int type, int si1, int sj1, `vrna_param_t *P`)
- `FLT_OR_DBL exp_E_ExtLoop` (int type, int si1, int sj1, `vrna_exp_param_t *P`)
- `int E_Stem` (int type, int si1, int sj1, int extLoop, `vrna_param_t *P`)
- `FLT_OR_DBL exp_E_Stem` (int type, int si1, int sj1, int extLoop, `vrna_exp_param_t *P`)

Energy evaluation of exterior loops for MFE and partition function calculations.

Read and write different file formats for RNA sequences, structures.

[illegible]

- Generated by Doxygen

Print a secondary structure as helix list.

- void [vrna_file_connect](#) (const char *seq, const char *db, float energy, const char *identifier, FILE *file)

Print a secondary structure as connect table.

- void [vrna_file_bpseq](#) (const char *seq, const char *db, FILE *file)

Print a secondary structure in bpseq format.

- void [vrna_file_json](#) (const char *seq, const char *db, double energy, const char *identifier, FILE *file)

Print a secondary structure in jsonformat.

- unsigned int [vrna_file_fasta_read_record](#) (char **header, char **sequence, char ***rest, FILE *file, unsigned int options)

Get a (fasta) data set from a file or stdin.

- char * [vrna_extract_record_rest_structure](#) (const char **lines, unsigned int length, unsigned int option)

Extract a dot-bracket structure string from (multiline)character array.

- int [vrna_file_SHAPE_read](#) (const char *file_name, int length, double default_value, char *sequence, double *values)

Read data from a given SHAPE reactivity input file.

- void [vrna_extract_record_rest_constraint](#) (char **cstruc, const char **lines, unsigned int option)

Extract a hard constraint encoded as pseudo dot-bracket string.

- unsigned int [read_record](#) (char **header, char **sequence, char ***rest, unsigned int options)

Get a data record from stdin.

17.28.1 Detailed Description

Read and write different file formats for RNA sequences, structures.

17.28.2 Macro Definition Documentation

17.28.2.1 `#define VRNA_OPTION_MULTILINE 32U`

Tell a function that an input is assumed to span several lines.

If used as input-option a function might also be returning this state telling that it has read data from multiple lines.

See also

[vrna_extract_record_rest_structure\(\)](#), [vrna_file_fasta_read_record\(\)](#)

17.28.2.2 `#define VRNA_CONSTRAINT_MULTILINE 32U`

parse multiline constraint

Deprecated see [vrna_extract_record_rest_structure\(\)](#)

17.28.3 Function Documentation

17.28.3.1 void `vrna_file_connect` (const char * *seq*, const char * *db*, float *energy*, const char * *identifier*, FILE * *file*)

Print a secondary structure as connect table.

Connect table file format looks like this:

```
300 ENERGY = 7.0 example
  1 G      0   2   22   1
  2 G      1   3   21   2
```

where the headerline is followed by 6 columns with:

1. Base number: index n
2. Base (A, C, G, T, U, X)
3. Index n-1 (0 if first nucleotide)
4. Index n+1 (0 if last nucleotide)
5. Number of the base to which n is paired. No pairing is indicated by 0 (zero).
6. Natural numbering.

Parameters

<i>seq</i>	The RNA sequence
<i>db</i>	The structure in dot-bracket format
<i>energy</i>	The free energy of the structure
<i>identifier</i>	An optional identifier for the sequence
<i>file</i>	The file handle used to print to (print defaults to 'stdout' if(file == NULL))

17.28.3.2 void `vrna_file_bpseq` (const char * *seq*, const char * *db*, FILE * *file*)

Print a secondary structure in bpseq format.

Parameters

<i>seq</i>	The RNA sequence
<i>db</i>	The structure in dot-bracket format
<i>file</i>	The file handle used to print to (print defaults to 'stdout' if(file == NULL))

17.28.3.3 void `vrna_file_json` (const char * *seq*, const char * *db*, double *energy*, const char * *identifier*, FILE * *file*)

Print a secondary structure in jsonformat.

Parameters

<i>seq</i>	The RNA sequence
<i>db</i>	The structure in dot-bracket format
<i>energy</i>	The free energy
<i>identifier</i>	An identifier for the sequence
<i>file</i>	The file handle used to print to (print defaults to 'stdout' if(file == NULL))

17.28.3.4 `unsigned int vrna_file_fasta_read_record (char ** header, char ** sequence, char *** rest, FILE * file, unsigned int options)`

Get a (fasta) data set from a file or stdin.

This function may be used to obtain complete datasets from a filehandle or stdin. A dataset is always defined to contain at least a sequence. If data starts with a fasta header, i.e. a line like

```
>some header info
```

then `vrna_file_fasta_read_record()` will assume that the sequence that follows the header may span over several lines. To disable this behavior and to assign a single line to the argument 'sequence' one can pass `VRNA_INPUT_NO_SPAN` in the 'options' argument. If no fasta header is read in the beginning of a data block, a sequence must not span over multiple lines!

Unless the options `VRNA_INPUT_NOSKIP_COMMENTS` or `VRNA_INPUT_NOSKIP_BLANK_LINES` are passed, a sequence may be interrupted by lines starting with a comment character or empty lines.

A sequence is regarded as completely read if it was either assumed to not span over multiple lines, a secondary structure or structure constraint follows the sequence on the next line, or a new header marks the beginning of a new sequence...

All lines following the sequence (this includes comments) that do not initiate a new dataset according to the above definition are available through the line-array 'rest'. Here one can usually find the structure constraint or other information belonging to the current dataset. Filling of 'rest' may be prevented by passing `VRNA_INPUT_NO_REST` to the options argument.

Note

This function will exit any program with an error message if no sequence could be read!

This function is NOT threadsafe! It uses a global variable to store information about the next data block.

The main purpose of this function is to be able to easily parse blocks of data in the header of a loop where all calculations for the appropriate data is done inside the loop. The loop may be then left on certain return values, e.g.:

```
00001 char *id, *seq, **rest;
00002 int i;
00003 id = seq = NULL;
00004 rest = NULL;
00005 while(! (vrna_file_fasta_read_record(&id, &seq, &rest, NULL, 0) & (VRNA_INPUT_ERROR |
VRNA_INPUT_QUIT))) {
00006     if(id) printf("%s\n", id);
00007     printf("%s\n", seq);
00008     if(rest)
00009         for(i=0; rest[i]; i++) {
00010             printf("%s\n", rest[i]);
00011             free(rest[i]);
00012         }
00013     free(rest);
00014     free(seq);
00015     free(id);
00016 }
```

In the example above, the while loop will be terminated when [vrna_file_fasta_read_record\(\)](#) returns either an error, EOF, or a user initiated quit request.

As long as data is read from stdin (we are passing NULL as the file pointer), the id is printed if it is available for the current block of data. The sequence will be printed in any case and if some more lines belong to the current block of data each line will be printed as well.

Note

Do not forget to free the memory occupied by header, sequence and rest!

Parameters

<i>header</i>	A pointer which will be set such that it points to the header of the record
<i>sequence</i>	A pointer which will be set such that it points to the sequence of the record
<i>rest</i>	A pointer which will be set such that it points to an array of lines which also belong to the record
<i>file</i>	A file handle to read from (if NULL, this function reads from stdin)
<i>options</i>	Some options which may be passed to alter the behavior of the function, use 0 for no options

Returns

A flag with information about what the function actually did read

17.28.3.5 `char* vrna_extract_record_rest_structure (const char ** lines, unsigned int length, unsigned int option)`

Extract a dot-bracket structure string from (multiline)character array.

This function extracts a dot-bracket structure string from the 'rest' array as returned by [vrna_file_fasta_read_record\(\)](#) and returns it. All occurrences of comments within the 'lines' array will be skipped as long as they do not break the structure string. If no structure could be read, this function returns NULL.

Precondition

The argument 'lines' has to be a 2-dimensional character array as obtained by [vrna_file_fasta_read_record\(\)](#)

See also

[vrna_file_fasta_read_record\(\)](#)

Parameters

<i>lines</i>	The (multiline) character array to be parsed
<i>length</i>	The assumed length of the dot-bracket string (passing a value < 1 results in no length limit)
<i>option</i>	Some options which may be passed to alter the behavior of the function, use 0 for no options

Returns

The dot-bracket string read from lines or NULL

17.28.3.6 `int vrna_file_SHAPE_read (const char * file_name, int length, double default_value, char * sequence, double * values)`

Read data from a given SHAPE reactivity input file.

This function parses the informations from a given file and stores the result in the preallocated string sequence and the double array values.

Parameters

<i>file_name</i>	Path to the constraints file
<i>length</i>	Length of the sequence (file entries exceeding this limit will cause an error)
<i>default_value</i>	Value for missing indices
<i>sequence</i>	Pointer to an array used for storing the sequence obtained from the SHAPE reactivity file
<i>values</i>	Pointer to an array used for storing the values obtained from the SHAPE reactivity file

17.28.3.7 `void vrna_extract_record_rest_constraint (char ** cstruc, const char ** lines, unsigned int option)`

Extract a hard constraint encoded as pseudo dot-bracket string.

Deprecated Use [vrna_extract_record_rest_structure\(\)](#) instead!

Precondition

The argument 'lines' has to be a 2-dimensional character array as obtained by [vrna_file_fasta_read_record\(\)](#)

See also

[vrna_file_fasta_read_record\(\)](#), [VRNA_CONSTRAINT_DB_PIPE](#), [VRNA_CONSTRAINT_DB_DOT](#), [VRNA_CONSTRAINT_DB_X](#) [VRNA_CONSTRAINT_DB_ANG_BRACK](#), [VRNA_CONSTRAINT_DB_RND_BRACK](#)

Parameters

<i>cstruc</i>	A pointer to a character array that is used as pseudo dot-bracket output
<i>lines</i>	A 2-dimensional character array with the extension lines from the FASTA input
<i>option</i>	The option flags that define the behavior and recognition pattern of this function

17.28.3.8 `unsigned int read_record (char ** header, char ** sequence, char *** rest, unsigned int options)`

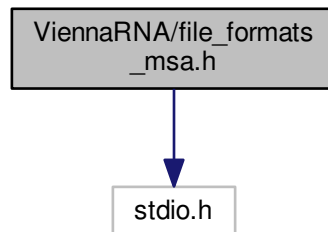
Get a data record from stdin.

Deprecated This function is deprecated! Use [vrna_file_fasta_read_record\(\)](#) as a replacment.

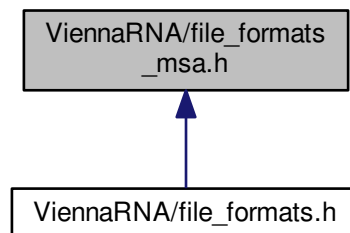
17.29 ViennaRNA/file_formats_msa.h File Reference

Functions dealing with file formats for Multiple Sequence Alignments (MSA)

Include dependency graph for file_formats_msa.h:



This graph shows which files directly or indirectly include this file:



Macros

- `#define VRNA_FILE_FORMAT_MSA_CLUSTAL 1U`
Option flag indicating ClustalW formatted files.
- `#define VRNA_FILE_FORMAT_MSA_STOCKHOLM 2U`
Option flag indicating Stockholm 1.0 formatted files.
- `#define VRNA_FILE_FORMAT_MSA_FASTA 4U`
Option flag indicating FASTA (Pearson) formatted files.
- `#define VRNA_FILE_FORMAT_MSA_MAF 8U`
Option flag indicating MAF formatted files.
- `#define VRNA_FILE_FORMAT_MSA_DEFAULT`
Option flag indicating the set of default file formats.
- `#define VRNA_FILE_FORMAT_MSA_NOCHECK 4096U`
Option flag to disable validation of the alignment.
- `#define VRNA_FILE_FORMAT_MSA_UNKNOWN 8192U`
Return flag of `vrna_file_msa_detect_format()` to indicate unknown or malformed alignment.

Functions

- int [vrna_file_msa_read](#) (const char *filename, char ***names, char ***aln, char **id, char **structure, unsigned int options)
Read a multiple sequence alignment from file.
- int [vrna_file_msa_read_record](#) (FILE *fp, char ***names, char ***aln, char **id, char **structure, unsigned int options)
Read a multiple sequence alignment from file handle.
- unsigned int [vrna_file_msa_detect_format](#) (const char *filename, unsigned int options)
Detect the format of a multiple sequence alignment file.

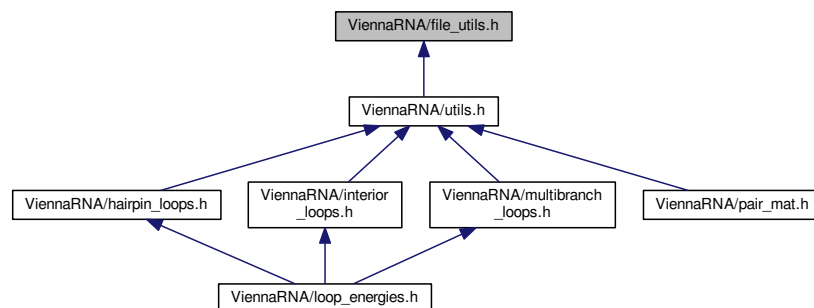
17.29.1 Detailed Description

Functions dealing with file formats for Multiple Sequence Alignments (MSA)

17.30 ViennaRNA/file_utils.h File Reference

Several utilities for file handling.

This graph shows which files directly or indirectly include this file:



Functions

- void [vrna_file_copy](#) (FILE *from, FILE *to)
Inefficient 'cp'.
- char * [vrna_read_line](#) (FILE *fp)
Read a line of arbitrary length from a stream.
- int [vrna_mkdir_p](#) (const char *path)
Recursively create a directory tree.
- char * [vrna_basename](#) (const char *path)
Extract the filename from a file path.
- char * [vrna_dirname](#) (const char *path)
Extract the directory part of a file path.

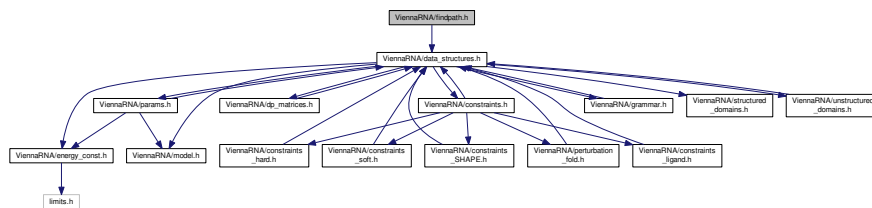
17.30.1 Detailed Description

Several utilities for file handling.

17.31 ViennaRNA/findpath.h File Reference

A breadth-first search heuristic for optimal direct folding paths.

Include dependency graph for findpath.h:



Data Structures

- struct [vrna_path_s](#)
An element of a refolding path list. [More...](#)

Typedefs

- typedef struct [vrna_path_s](#) [vrna_path_t](#)
Typename for the refolding path data structure [vrna_path_s](#).
- typedef struct [vrna_path_s](#) [path_t](#)
Old typename of [vrna_path_s](#).

Functions

- int [vrna_path_findpath_saddle](#) ([vrna_fold_compound_t](#) *vc, const char *struc1, const char *struc2, int max)
Find energy of a saddle point between 2 structures (search only direct path)
- [vrna_path_t](#) * [vrna_path_findpath](#) ([vrna_fold_compound_t](#) *vc, const char *s1, const char *s2, int maxkeep)
Find refolding path between 2 structures (search only direct path)
- int [find_saddle](#) (const char *seq, const char *struc1, const char *struc2, int max)
Find energy of a saddle point between 2 structures (search only direct path)
- void [free_path](#) ([vrna_path_t](#) *path)
Free memory allocated by [get_path\(\)](#) function.
- [vrna_path_t](#) * [get_path](#) (const char *seq, const char *s1, const char *s2, int maxkeep)
Find refolding path between 2 structures (search only direct path)

17.31.1 Detailed Description

A breadth-first search heuristic for optimal direct folding paths.

17.33.1 Detailed Description

Here all all declarations of the global variables used throughout RNAlib.

17.33.2 Variable Documentation

17.33.2.1 `char* RibosumFile`

warning this variable will vanish in the future ribosums will be compiled in instead

17.33.2.2 `int james_rule`

interior loops of size 2 get energy 0.8Kcal and no mismatches, default 1

17.33.2.3 `int logML`

use logarithmic multiloop energy function

17.33.2.4 `int cut_point`

Marks the position (starting from 1) of the first nucleotide of the second molecule within the concatenated sequence.

To evaluate the energy of a duplex structure (a structure formed by two strands), concatenate the to sequences and set it to the first base of the second strand in the concatenated sequence. The default value of -1 stands for single molecule folding. The `cut_point` variable is also used by [vrna_file_PS_rnaplot\(\)](#) and [PS_dot_plot\(\)](#) to mark the chain break in postscript plots.

17.33.2.5 `bondT* base_pair`

Contains a list of base pairs after a call to [fold\(\)](#).

`base_pair[0].i` contains the total number of pairs.

Deprecated Do not use this variable anymore!

17.33.2.6 `FLT_OR_DBL* pr`

A pointer to the base pair probability matrix.

Deprecated Do not use this variable anymore!

17.33.2.7 int* iindx

index array to move through pr.

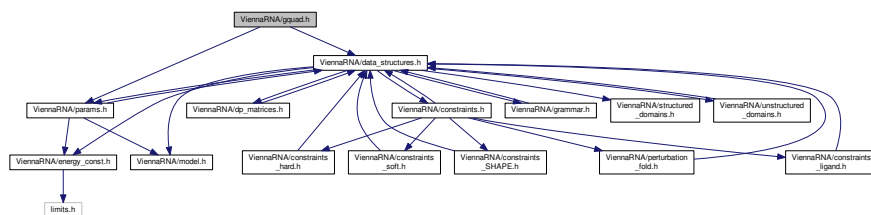
The probability for base i and j to form a pair is in pr[iindx[i]-j].

Deprecated Do not use this variable anymore!

17.34 ViennaRNA/gquad.h File Reference

G-quadruplexes.

Include dependency graph for gquad.h:



Functions

- int * [get_gquad_matrix](#) (short *S, [vrna_param_t](#) *P)
Get a triangular matrix prefilled with minimum free energy contributions of G-quadruplexes.
- int [parse_gquad](#) (const char *struc, int *L, int l[3])
- PRIVATE int [backtrack_GQuad_IntLoop](#) (int c, int i, int j, int type, short *S, int *ggg, int *index, int *p, int *q, [vrna_param_t](#) *P)
- PRIVATE int [backtrack_GQuad_IntLoop_L](#) (int c, int i, int j, int type, short *S, int **ggg, int maxdist, int *p, int *q, [vrna_param_t](#) *P)

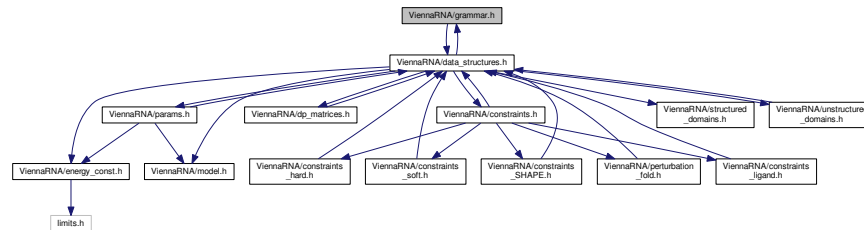
17.34.1 Detailed Description

G-quadruplexes.

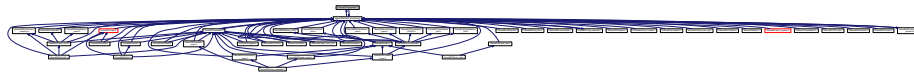
17.35 ViennaRNA/grammar.h File Reference

Implementations for the RNA folding grammar.

Include dependency graph for grammar.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [vrna_gr_aux_s](#)

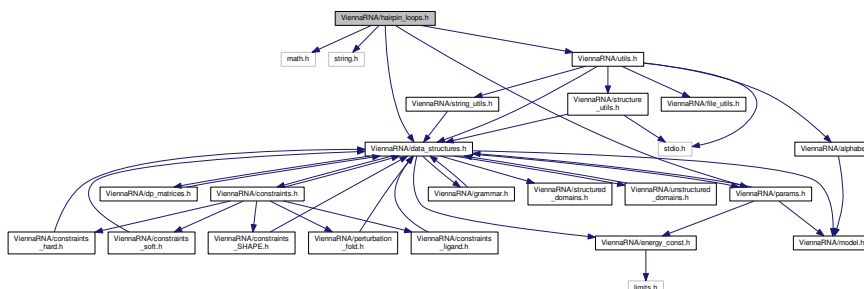
17.35.1 Detailed Description

Implementations for the RNA folding grammar.

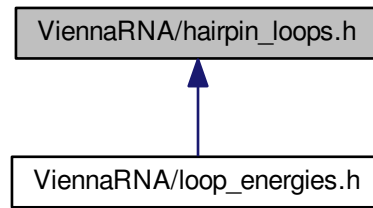
17.36 ViennaRNA/hairpin_loops.h File Reference

Energy evaluation of hairpin loops for MFE and partition function calculations.

Include dependency graph for hairpin_loops.h:



This graph shows which files directly or indirectly include this file:



Functions

- PRIVATE int [E_Hairpin](#) (int size, int type, int si1, int sj1, const char *string, [vrna_param_t](#) *P)
Compute the Energy of a hairpin-loop.
- PRIVATE [FLT_OR_DBL exp_E_Hairpin](#) (int u, int type, short si1, short sj1, const char *string, [vrna_exp_param_t](#) *P)
Compute Boltzmann weight $e^{-\Delta G/kT}$ of a hairpin loop.
- int [vrna_E_hp_loop](#) ([vrna_fold_compound_t](#) *vc, int i, int j)
Evaluate the free energy of a hairpin loop and consider hard constraints if they apply.
- int [vrna_E_ext_hp_loop](#) ([vrna_fold_compound_t](#) *vc, int i, int j)
Evaluate the free energy of an exterior hairpin loop and consider possible hard constraints.
- int [vrna_eval_ext_hp_loop](#) ([vrna_fold_compound_t](#) *vc, int i, int j)
Evaluate free energy of an exterior hairpin loop.
- int [vrna_eval_hp_loop](#) ([vrna_fold_compound_t](#) *vc, int i, int j)
Evaluate free energy of a hairpin loop.
- [FLT_OR_DBL vrna_exp_E_hp_loop](#) ([vrna_fold_compound_t](#) *vc, int i, int j)
High-Level function for hairpin loop energy evaluation (partition function variant)
- int [vrna_BT_hp_loop](#) ([vrna_fold_compound_t](#) *vc, int i, int j, int en, [vrna_bp_stack_t](#) *bp_stack, int *stack_count)
Backtrack a hairpin loop closed by (i, j) .

17.36.1 Detailed Description

Energy evaluation of hairpin loops for MFE and partition function calculations.

17.37 ViennaRNA/interior_loops.h File Reference

Energy evaluation of interior loops for MFE and partition function calculations.

Functions

- float [inverse_fold](#) (char *start, const char *target)
Find sequences with predefined structure.
- float [inverse_pf_fold](#) (char *start, const char *target)
Find sequence that maximizes probability of a predefined structure.

Variables

- char * [symbolset](#)
This global variable points to the allowed bases, initially "AUGC". It can be used to design sequences from reduced alphabets.
- float [final_cost](#)
- int [give_up](#)
- int [inv_verbose](#)

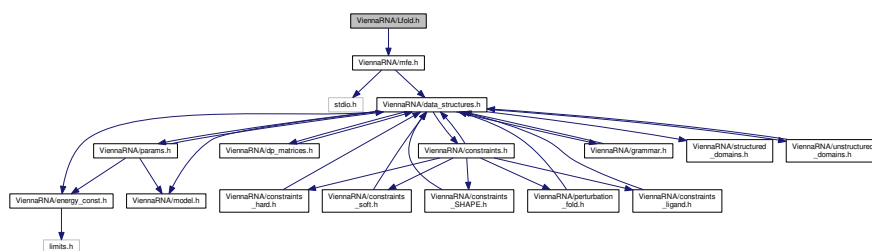
17.38.1 Detailed Description

Inverse folding routines.

17.39 ViennaRNA/Lfold.h File Reference

Functions for locally optimal MFE structure prediction.

Include dependency graph for Lfold.h:



Functions

- float [vrna_Lfold](#) (const char *string, int window_size, FILE *file)
Local MFE prediction using a sliding window approach (simplified interface)
- float [vrna_Lfoldz](#) (const char *string, int window_size, double min_z, FILE *file)
Local MFE prediction using a sliding window approach with z-score cut-off (simplified interface)
- float [aliLfold](#) (const char **strings, char *structure, int maxdist)
- float [Lfold](#) (const char *string, char *structure, int maxdist)
The local analog to fold().
- float [Lfoldz](#) (const char *string, char *structure, int maxdist, int zsc, double min_z)

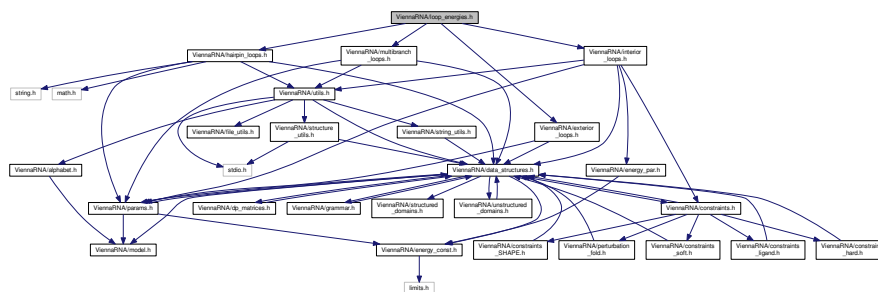
17.39.1 Detailed Description

Functions for locally optimal MFE structure prediction.

17.40 ViennaRNA/loop_energies.h File Reference

Energy evaluation for MFE and partition function calculations.

Include dependency graph for loop_energies.h:



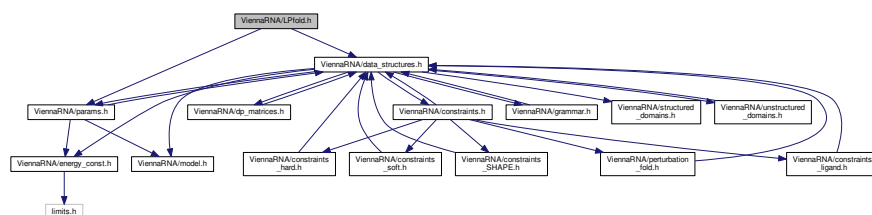
17.40.1 Detailed Description

Energy evaluation for MFE and partition function calculations.

17.41 ViennaRNA/LPfold.h File Reference

Partition function implementation for the Lfold algorithm.

Include dependency graph for LPfold.h:



Functions

- void [update_pf_paramsLP](#) (int length)
- [plist](#) * [pfl_fold](#) (char *sequence, int winSize, int pairSize, float cutoffb, double **pU, [plist](#) **dpp2, FILE *pUfp, FILE *spup)
Compute partition functions for locally stable secondary structures.
- [plist](#) * [pfl_fold_par](#) (char *sequence, int winSize, int pairSize, float cutoffb, double **pU, [plist](#) **dpp2, FILE *pUfp, FILE *spup, [vrna_exp_param_t](#) *parameters)
Compute partition functions for locally stable secondary structures.
- void [putoutpU_prob](#) (double **pU, int length, int ulength, FILE *fp, int energies)
Writes the unpaired probabilities (pU) or opening energies into a file.
- void [putoutpU_prob_bin](#) (double **pU, int length, int ulength, FILE *fp, int energies)
Writes the unpaired probabilities (pU) or opening energies into a binary file.
- void [init_pf_foldLP](#) (int length)

17.41.1 Detailed Description

Partition function implementation for the Lfold algorithm.

17.41.2 Function Documentation

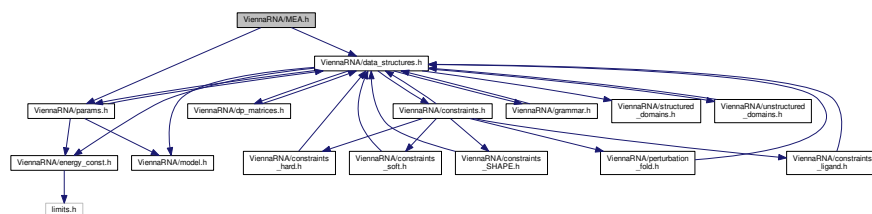
17.41.2.1 void [init_pf_foldLP](#) (int length)

Dunno if this function was ever used by external programs linking to RNAlib, but it was declared PUBLIC before. Anyway, never use this function as it will be removed soon and does nothing at all

17.42 ViennaRNA/MEA.h File Reference

Computes a MEA (maximum expected accuracy) structure.

Include dependency graph for MEA.h:



Functions

- float [MEA](#) ([plist](#) *p, char *structure, double gamma)
Computes a MEA (maximum expected accuracy) structure.

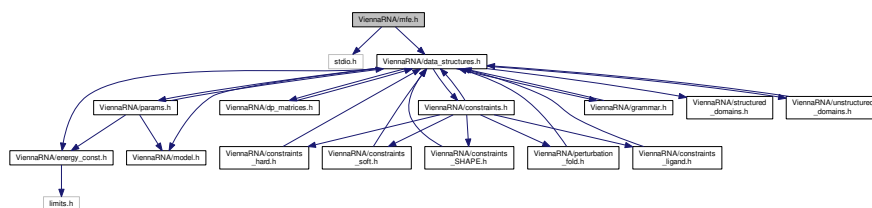
17.42.1 Detailed Description

Computes a MEA (maximum expected accuracy) structure.

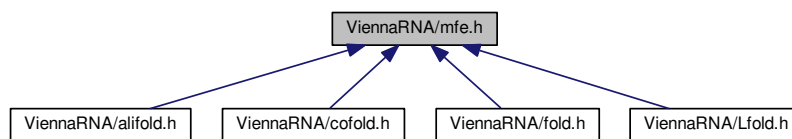
17.43 ViennaRNA/mfe.h File Reference

MFE calculations for single RNA sequences.

Include dependency graph for mfe.h:



This graph shows which files directly or indirectly include this file:



Functions

- float [vrna_mfe](#) ([vrna_fold_compound_t](#) *vc, char *structure)
Compute minimum free energy and an appropriate secondary structure of an RNA sequence, or RNA sequence alignment.
- float [vrna_mfe_dimer](#) ([vrna_fold_compound_t](#) *vc, char *structure)
Compute the minimum free energy of two interacting RNA molecules.
- float [vrna_mfe_window](#) ([vrna_fold_compound_t](#) *vc, FILE *file)
Local MFE prediction using a sliding window approach.
- float [vrna_mfe_window_zscore](#) ([vrna_fold_compound_t](#) *vc, double min_z, FILE *file)
Local MFE prediction using a sliding window approach (with z-score cut-off)

17.43.1 Detailed Description

MFE calculations for single RNA sequences.

This file includes (almost) all function declarations within the RNAlib that are related to MFE folding...

17.44 ViennaRNA/mm.h File Reference

Several Maximum Matching implementations.

17.44.1 Detailed Description

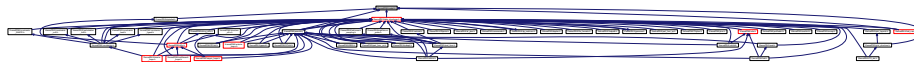
Several Maximum Matching implementations.

This file contains the declarations for several maximum matching implementations

17.45 ViennaRNA/model.h File Reference

The model details data structure and its corresponding modifiers.

This graph shows which files directly or indirectly include this file:



Data Structures

- struct [vrna_md_s](#)

The data structure that contains the complete model details used throughout the calculations.

- #define [VRNA_MODEL_DEFAULT_TEMPERATURE](#) 37.0
Default temperature for structure prediction and free energy evaluation in °C
- #define [VRNA_MODEL_DEFAULT_PF_SCALE](#) -1
Default scaling factor for partition function computations.
- #define [VRNA_MODEL_DEFAULT_BETA_SCALE](#) 1.
Default scaling factor for absolute thermodynamic temperature in Boltzmann factors.
- #define [VRNA_MODEL_DEFAULT_DANGLES](#) 2
Default dangling end model.
- #define [VRNA_MODEL_DEFAULT_SPECIAL_HP](#) 1
Default model behavior for lookup of special tri-, tetra-, and hexa-loops.
- #define [VRNA_MODEL_DEFAULT_NO_LP](#) 0
Default model behavior for so-called 'lonely pairs'.
- #define [VRNA_MODEL_DEFAULT_NO_GU](#) 0
Default model behavior for G-U base pairs.
- #define [VRNA_MODEL_DEFAULT_NO_GU_CLOSURE](#) 0
Default model behavior for G-U base pairs closing a loop.
- #define [VRNA_MODEL_DEFAULT_CIRC](#) 0
Default model behavior to treat a molecule as a circular RNA (DNA)
- #define [VRNA_MODEL_DEFAULT_GQUAD](#) 0
Default model behavior regarding the treatment of G-Quadruplexes.
- #define [VRNA_MODEL_DEFAULT_UNIQ_ML](#) 0
Default behavior of the model regarding unique multi-branch loop decomposition.

- `#define VRNA_MODEL_DEFAULT_ENERGY_SET 0`
Default model behavior on which energy set to use.
- `#define VRNA_MODEL_DEFAULT_BACKTRACK 1`
Default model behavior with regards to backtracking of structures.
- `#define VRNA_MODEL_DEFAULT_BACKTRACK_TYPE 'F'`
Default model behavior on what type of backtracking to perform.
- `#define VRNA_MODEL_DEFAULT_COMPUTE_BPP 1`
Default model behavior with regards to computing base pair probabilities.
- `#define VRNA_MODEL_DEFAULT_MAX_BP_SPAN -1`
Default model behavior for the allowed maximum base pair span.
- `#define VRNA_MODEL_DEFAULT_WINDOW_SIZE -1`
Default model behavior for the sliding window approach.
- `#define VRNA_MODEL_DEFAULT_LOG_ML 0`
Default model behavior on how to evaluate the energy contribution of multi-branch loops.
- `#define VRNA_MODEL_DEFAULT_ALI_OLD_EN 0`
Default model behavior for consensus structure energy evaluation.
- `#define VRNA_MODEL_DEFAULT_ALI_RIBO 0`
Default model behavior for consensus structure co-variance contribution assessment.
- `#define VRNA_MODEL_DEFAULT_ALI_CV_FACT 1.`
Default model behavior for weighting the co-variance score in consensus structure prediction.
- `#define VRNA_MODEL_DEFAULT_ALI_NC_FACT 1.`
Default model behavior for weighting the nucleotide conservation? in consensus structure prediction.
- `#define MAXALPHA 20`
Maximal length of alphabet.
- `typedef struct vrna_md_s vrna_md_t`
Typename for the model details data structure `vrna_md_s`.
- `double temperature`
Rescale energy parameters to a temperature in degC.
- `double pf_scale`
A scaling factor used by `pf_fold()` to avoid overflows.
- `int dangles`
Switch the energy model for dangling end contributions (0, 1, 2, 3)
- `int tetra_loop`
Include special stabilizing energies for some tri-, tetra- and hexa-loops;.
- `int noLonelyPairs`
Global switch to avoid/allow helices of length 1.
- `int noGU`
Global switch to forbid/allow GU base pairs at all.
- `int no_closingGU`
GU allowed only inside stacks if set to 1.
- `int circ`
backward compatibility variable.. this does not effect anything
- `int gquad`
Allow G-quadruplex formation.
- `int canonicalBPOnly`
- `int uniq_ML`
do ML decomposition uniquely (for subopt)
- `int energy_set`
0 = BP; 1=any with GC; 2=any with AU-parameter
- `int do_backtrack`
do backtracking, i.e. compute secondary structures or base pair probabilities

- char [backtrack_type](#)
A backtrack array marker for [inverse_fold\(\)](#)
- char * [nonstandards](#)
contains allowed non standard base pairs
- int [max_bp_span](#)
Maximum allowed base pair span.
- int [oldAliEn](#)
use old alifold energies (with gaps)
- int [ribo](#)
use ribosum matrices
- int [logML](#)
if nonzero use logarithmic ML energy in [energy_of_struct](#)
- void [vrna_md_set_default](#) ([vrna_md_t](#) *md)
Apply default model details to a provided [vrna_md_t](#) data structure.
- void [vrna_md_update](#) ([vrna_md_t](#) *md)
Update the model details data structure.
- [vrna_md_t](#) * [vrna_md_copy](#) ([vrna_md_t](#) *md_to, const [vrna_md_t](#) *md_from)
Copy/Clone a [vrna_md_t](#) model.
- char * [vrna_md_option_string](#) ([vrna_md_t](#) *md)
Get a corresponding commandline parameter string of the options in a [vrna_md_t](#).
- void [vrna_md_defaults_reset](#) ([vrna_md_t](#) *md_p)
Reset the global default model details to a specific set of parameters, or their initial values.
- void [vrna_md_defaults_temperature](#) (double T)
Set default temperature for energy evaluation of loops.
- double [vrna_md_defaults_temperature_get](#) (void)
Get default temperature for energy evaluation of loops.
- void [vrna_md_defaults_betaScale](#) (double b)
Set default scaling factor of thermodynamic temperature in Boltzmann factors.
- double [vrna_md_defaults_betaScale_get](#) (void)
Get default scaling factor of thermodynamic temperature in Boltzmann factors.
- void [vrna_md_defaults_dangles](#) (int d)
Set default dangle model for structure prediction.
- int [vrna_md_defaults_dangles_get](#) (void)
Get default dangle model for structure prediction.
- void [vrna_md_defaults_special_hp](#) (int flag)
Set default behavior for lookup of tabulated free energies for special hairpin loops, such as Tri-, Tetra-, or Hexa-loops.
- int [vrna_md_defaults_special_hp_get](#) (void)
Get default behavior for lookup of tabulated free energies for special hairpin loops, such as Tri-, Tetra-, or Hexa-loops.
- void [vrna_md_defaults_noLP](#) (int flag)
Set default behavior for prediction of canonical secondary structures.
- int [vrna_md_defaults_noLP_get](#) (void)
Get default behavior for prediction of canonical secondary structures.
- void [vrna_md_defaults_noGU](#) (int flag)
Set default behavior for treatment of G-U wobble pairs.
- int [vrna_md_defaults_noGU_get](#) (void)
Get default behavior for treatment of G-U wobble pairs.
- void [vrna_md_defaults_noGUclosure](#) (int flag)
Set default behavior for G-U pairs as closing pair for loops.
- int [vrna_md_defaults_noGUclosure_get](#) (void)
Get default behavior for G-U pairs as closing pair for loops.
- void [vrna_md_defaults_logML](#) (int flag)

- Set default behavior recomputing free energies of multi-branch loops using a logarithmic model.*

 - int [vrna_md_defaults_logML_get](#) (void)

Get default behavior recomputing free energies of multi-branch loops using a logarithmic model.
- void [vrna_md_defaults_circ](#) (int flag)

Set default behavior whether input sequences are circularized.

 - int [vrna_md_defaults_circ_get](#) (void)

Get default behavior whether input sequences are circularized.
- void [vrna_md_defaults_gquad](#) (int flag)

Set default behavior for treatment of G-Quadruplexes.

 - int [vrna_md_defaults_gquad_get](#) (void)

Get default behavior for treatment of G-Quadruplexes.
- void [vrna_md_defaults_uniq_ML](#) (int flag)

Set default behavior for creating additional matrix for unique multi-branch loop prediction.

 - int [vrna_md_defaults_uniq_ML_get](#) (void)

Get default behavior for creating additional matrix for unique multi-branch loop prediction.
- void [vrna_md_defaults_energy_set](#) (int e)

Set default energy set.

 - int [vrna_md_defaults_energy_set_get](#) (void)

Get default energy set.
- void [vrna_md_defaults_backtrack](#) (int flag)

Set default behavior for whether to backtrack secondary structures.

 - int [vrna_md_defaults_backtrack_get](#) (void)

Get default behavior for whether to backtrack secondary structures.
- void [vrna_md_defaults_backtrack_type](#) (char t)

Set default backtrack type, i.e. which DP matrix is used.

 - char [vrna_md_defaults_backtrack_type_get](#) (void)

Get default backtrack type, i.e. which DP matrix is used.
- void [vrna_md_defaults_compute_bpp](#) (int flag)

Set the default behavior for whether to compute base pair probabilities after partition function computation.

 - int [vrna_md_defaults_compute_bpp_get](#) (void)

Get the default behavior for whether to compute base pair probabilities after partition function computation.
- void [vrna_md_defaults_max_bp_span](#) (int span)

Set default maximal base pair span.

 - int [vrna_md_defaults_max_bp_span_get](#) (void)

Get default maximal base pair span.
- void [vrna_md_defaults_min_loop_size](#) (int size)

Set default minimal loop size.

 - int [vrna_md_defaults_min_loop_size_get](#) (void)

Get default minimal loop size.
- void [vrna_md_defaults_window_size](#) (int size)

Set default window size for sliding window structure prediction approaches.

 - int [vrna_md_defaults_window_size_get](#) (void)

Get default window size for sliding window structure prediction approaches.
- void [vrna_md_defaults_oldAliEn](#) (int flag)

Set default behavior for whether to use old energy model for comparative structure prediction.

 - int [vrna_md_defaults_oldAliEn_get](#) (void)

Get default behavior for whether to use old energy model for comparative structure prediction.
- void [vrna_md_defaults_ribo](#) (int flag)

Set default behavior for whether to use Ribosum Scoring in comparative structure prediction.

 - int [vrna_md_defaults_ribo_get](#) (void)

Get default behavior for whether to use Ribosum Scoring in comparative structure prediction.

- void [vrna_md_defaults_cv_fact](#) (double factor)
Set the default co-variance scaling factor used in comparative structure prediction.
- double [vrna_md_defaults_cv_fact_get](#) (void)
Get the default co-variance scaling factor used in comparative structure prediction.
- void [vrna_md_defaults_nc_fact](#) (double factor)
- double [vrna_md_defaults_nc_fact_get](#) (void)
- void [vrna_md_defaults_sfact](#) (double factor)
Set the default scaling factor used to avoid under-/overflows in partition function computation.
- double [vrna_md_defaults_sfact_get](#) (void)
Get the default scaling factor used to avoid under-/overflows in partition function computation.
- void [set_model_details](#) ([vrna_md_t](#) *md)
Set default model details.

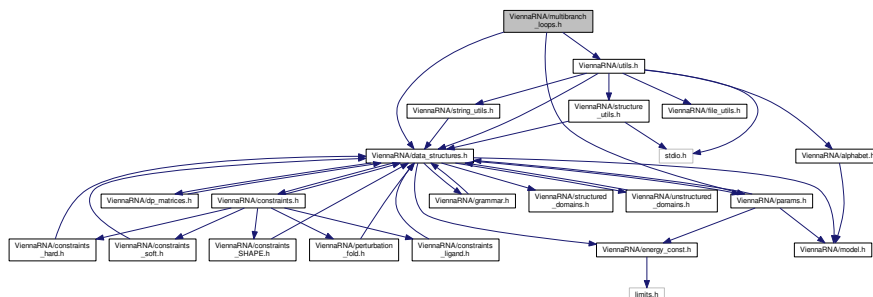
17.45.1 Detailed Description

The model details data structure and its corresponding modifiers.

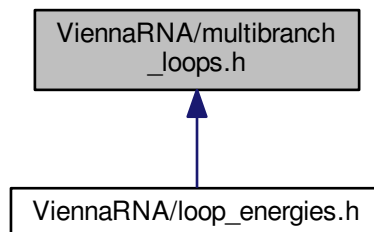
17.46 ViennaRNA/multibranch_loops.h File Reference

Energy evaluation of multibranch loops for MFE and partition function calculations.

Include dependency graph for multibranch_loops.h:



This graph shows which files directly or indirectly include this file:



Functions

- int `E_mb_loop_stack` (int *i*, int *j*, `vrna_fold_compound_t` **vc*)
Evaluate energy of a multi branch helices stacking onto closing pair (i,j)
- int `vrna_BT_mb_loop` (`vrna_fold_compound_t` **vc*, int **i*, int **j*, int **k*, int *en*, int **component1*, int **component2*)
Backtrack the decomposition of a multi branch loop closed by (i,j).

17.46.1 Detailed Description

Energy evaluation of multibranch loops for MFE and partition function calculations.

17.46.2 Function Documentation

17.46.2.1 int `E_mb_loop_stack` (int *i*, int *j*, `vrna_fold_compound_t` * *vc*)

Evaluate energy of a multi branch helices stacking onto closing pair (i,j)

Computes total free energy for coaxial stacking of (i,j) with (i+1.k) or (k+1.j-1)

17.46.2.2 int `vrna_BT_mb_loop` (`vrna_fold_compound_t` * *vc*, int * *i*, int * *j*, int * *k*, int *en*, int * *component1*, int * *component2*)

Backtrack the decomposition of a multi branch loop closed by (i,j).

Parameters

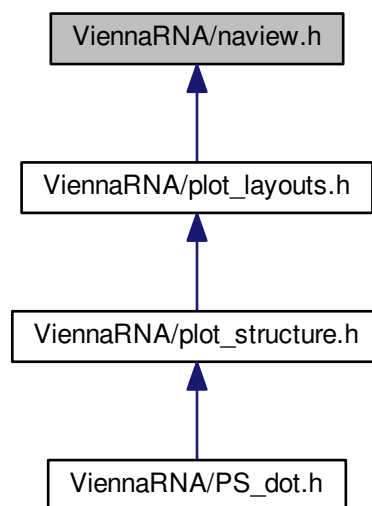
<i>vc</i>	The <code>vrna_fold_compound_t</code> filled with all relevant data for backtracking
<i>i</i>	5' position of base pair closing the loop (will be set to 5' position of leftmost decomposed block upon successful backtracking)
<i>j</i>	3' position of base pair closing the loop (will be set to 3' position of rightmost decomposed block upon successful backtracking)
<i>k</i>	Split position that delimits leftmost from rightmost block, [<i>i</i> , <i>k</i>] and [<i>k</i> +1, <i>j</i>], respectively. (Will be set upon successful backtracking)
<i>en</i>	The energy contribution of the substructure enclosed by (i,j)
<i>component1</i>	Type of leftmost block (1 = ML, 2 = C)
<i>component2</i>	Type of rightmost block (1 = ML, 2 = C)

Returns

1, if backtracking succeeded, 0 otherwise.

17.47 ViennaRNA/naview.h File Reference

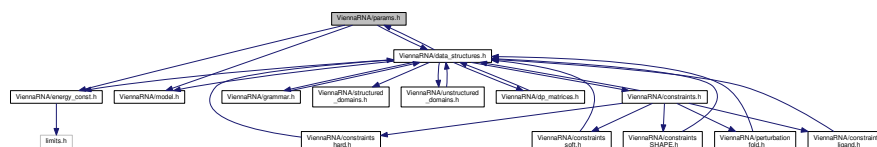
This graph shows which files directly or indirectly include this file:



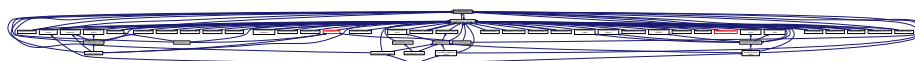
17.48 ViennaRNA/params.h File Reference

Functions to deal with sets of energy parameters.

Include dependency graph for params.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [vrna_param_s](#)
The datastructure that contains temperature scaled energy parameters. [More...](#)
- struct [vrna_exp_param_s](#)
The data structure that contains temperature scaled Boltzmann weights of the energy parameters. [More...](#)

Typedefs

- typedef struct [vrna_param_s](#) [vrna_param_t](#)
Typename for the free energy parameter data structure [vrna_params](#).
- typedef struct [vrna_exp_param_s](#) [vrna_exp_param_t](#)
Typename for the Boltzmann factor data structure [vrna_exp_params](#).
- typedef struct [vrna_param_s](#) paramT
Old typename of [vrna_param_s](#).
- typedef struct [vrna_exp_param_s](#) pf_paramT
Old typename of [vrna_exp_param_s](#).

Functions

- [vrna_param_t](#) * [vrna_params](#) ([vrna_md_t](#) *md)
Get a data structure containing prescaled free energy parameters.
- [vrna_param_t](#) * [vrna_params_copy](#) ([vrna_param_t](#) *par)
Get a copy of the provided free energy parameters.
- [vrna_exp_param_t](#) * [vrna_exp_params](#) ([vrna_md_t](#) *md)
Get a data structure containing prescaled free energy parameters already transformed to Boltzmann factors.
- [vrna_exp_param_t](#) * [vrna_exp_params_comparative](#) (unsigned int n_seq, [vrna_md_t](#) *md)
Get a data structure containing prescaled free energy parameters already transformed to Boltzmann factors (alifold version)
- [vrna_exp_param_t](#) * [vrna_exp_params_copy](#) ([vrna_exp_param_t](#) *par)
Get a copy of the provided free energy parameters (provided as Boltzmann factors)
- void [vrna_params_subst](#) ([vrna_fold_compound_t](#) *vc, [vrna_param_t](#) *par)
Update/Reset energy parameters data structure within a [vrna_fold_compound_t](#).
- void [vrna_exp_params_subst](#) ([vrna_fold_compound_t](#) *vc, [vrna_exp_param_t](#) *params)
Update the energy parameters for subsequent partition function computations.
- void [vrna_exp_params_rescale](#) ([vrna_fold_compound_t](#) *vc, double *mfe)
Rescale Boltzmann factors for partition function computations.
- void [vrna_params_reset](#) ([vrna_fold_compound_t](#) *vc, [vrna_md_t](#) *md_p)
Reset free energy parameters within a [vrna_fold_compound_t](#) according to provided, or default model details.
- void [vrna_exp_params_reset](#) ([vrna_fold_compound_t](#) *vc, [vrna_md_t](#) *md_p)
Reset Boltzmann factors for partition function computations within a [vrna_fold_compound_t](#) according to provided, or default model details.
- [vrna_exp_param_t](#) * [get_scaled_pf_parameters](#) (void)
Get precomputed Boltzmann factors of the loop type dependent energy contributions with independent thermodynamic temperature.
- [vrna_exp_param_t](#) * [get_boltzmann_factors](#) (double temperature, double betaScale, [vrna_md_t](#) md, double pf_scale)
Get precomputed Boltzmann factors of the loop type dependent energy contributions with independent thermodynamic temperature.
- [vrna_exp_param_t](#) * [get_boltzmann_factor_copy](#) ([vrna_exp_param_t](#) *parameters)
Get a copy of already precomputed Boltzmann factors.
- [vrna_exp_param_t](#) * [get_scaled_alipf_parameters](#) (unsigned int n_seq)

- `vrna_exp_param_t * get_boltzmann_factors_ali` (unsigned int `n_seq`, double `temperature`, double `betaScale`, `vrna_md_t` `md`, double `pf_scale`)

- `vrna_param_t * scale_parameters` (void)

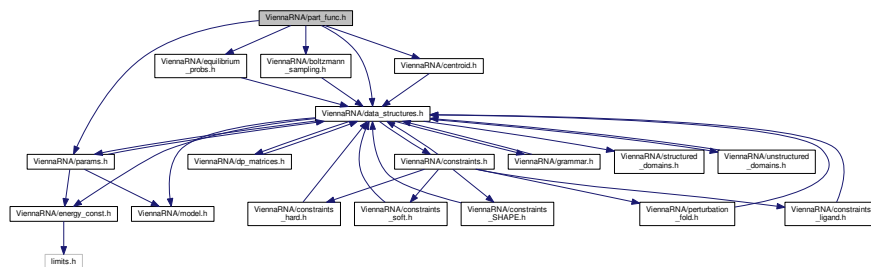
- `vrna_param_t * get_scaled_parameters (double temperature, vrna_md_t md)`

Get precomputed energy contributions for all the known loop types.

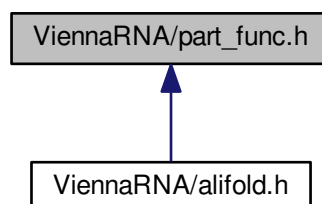
Functions to deal with sets of energy parameters.

Partition function implementations.

Include dependency graph for part_func.h:



This graph shows which files directly or indirectly include this file:



Functions

- float [vrna_pf](#) ([vrna_fold_compound_t](#) *vc, char *structure)
Compute the partition function Q for a given RNA sequence, or sequence alignment.
- float [vrna_pf_fold](#) (const char *sequence, char *structure, [vrna_plist_t](#) **pl)
Compute Partition function Q (and base pair probabilities) for an RNA sequence using a comparative method.
- float [vrna_pf_circfold](#) (const char *sequence, char *structure, [vrna_plist_t](#) **pl)
Compute Partition function Q (and base pair probabilities) for a circular RNA sequences using a comparative method.
- int [vrna_pf_float_precision](#) (void)
Find out whether partition function computations are using single precision floating points.
- float [pf_fold_par](#) (const char *sequence, char *structure, [vrna_exp_param_t](#) *parameters, int calculate_↵
bppm, int is_constrained, int is_circular)
Compute the partition function Q for a given RNA sequence.
- float [pf_fold](#) (const char *sequence, char *structure)
Compute the partition function Q of an RNA sequence.
- float [pf_circ_fold](#) (const char *sequence, char *structure)
Compute the partition function of a circular RNA sequence.
- char * [pbacktrack](#) (char *sequence)
Sample a secondary structure from the Boltzmann ensemble according its probability.
- char * [pbacktrack_circ](#) (char *sequence)
Sample a secondary structure of a circular RNA from the Boltzmann ensemble according its probability.
- void [free_pf_arrays](#) (void)
Free arrays for the partition function recursions.
- void [update_pf_params](#) (int length)
Recalculate energy parameters.
- void [update_pf_params_par](#) (int length, [vrna_exp_param_t](#) *parameters)
Recalculate energy parameters.
- [FLT_OR_DBL](#) * [export_bppm](#) (void)
*Get a pointer to the base pair probability array
Accessing the base pair probabilities for a pair (i,j) is achieved by.*
- int [get_pf_arrays](#) (short **S_p, short **S1_p, char **ptype_p, [FLT_OR_DBL](#) **qb_p, [FLT_OR_DBL](#) **qm↵
_p, [FLT_OR_DBL](#) **q1k_p, [FLT_OR_DBL](#) **qln_p)
Get the pointers to (almost) all relevant computation arrays used in partition function computation.
- double [get_subseq_F](#) (int i, int j)
Get the free energy of a subsequence from the q[] array.
- double [mean_bp_distance](#) (int length)
Get the mean base pair distance of the last partition function computation.
- double [mean_bp_distance_pr](#) (int length, [FLT_OR_DBL](#) *pr)
Get the mean base pair distance in the thermodynamic ensemble.
- [vrna_plist_t](#) * [stackProb](#) (double cutoff)
Get the probability of stacks.
- void [init_pf_fold](#) (int length)
Allocate space for [pf_fold\(\)](#)
- char * [centroid](#) (int length, double *dist)
- char * [get_centroid_struct_gquad_pr](#) (int length, double *dist)
- double [mean_bp_dist](#) (int length)
- double [expLoopEnergy](#) (int u1, int u2, int type, int type2, short si1, short sj1, short sp1, short sq1)
- double [expHairpinEnergy](#) (int u, int type, short si1, short sj1, const char *string)

Variables

- `int st_back`

Flag indicating that auxiliary arrays are needed throughout the computations. This is essential for stochastic backtracking.

17.49.1 Detailed Description

Partition function implementations.

This file includes (almost) all function declarations within the **RNALib** that are related to Partition function folding...

17.49.2 Function Documentation

17.49.2.1 `int vrna_pf_float_precision (void)`

Find out whether partition function computations are using single precision floating points.

See also

[FLT_OR_DBL](#)

Returns

1 if single precision is used, 0 otherwise

17.49.2.2 `vrna_plist_t* stackProb (double cutoff)`

Get the probability of stacks.

Deprecated Use `vrna_stack_prob()` instead!

17.49.2.3 `void init_pf_fold (int length)`

Allocate space for `pf_fold()`

Deprecated This function is obsolete and will be removed soon!

17.49.2.4 `char* centroid (int length, double * dist)`

Deprecated This function is deprecated and should not be used anymore as it is not threadsafe!

See also

[get_centroid_struct_pl\(\)](#), [get_centroid_struct_pr\(\)](#)

17.49.2.5 `char* get_centroid_struct_gquad_pr (int length, double * dist)`

Deprecated This function is deprecated and should not be used anymore as it is not threadsafe!

See also

[vrna_centroid\(\)](#), [vrna_centroid_from_probs\(\)](#), [vrna_centroid_from_plist\(\)](#)

17.49.2.6 `double mean_bp_dist (int length)`

get the mean pair distance of ensemble

Deprecated This function is not threadsafe and should not be used anymore. Use [mean_bp_distance\(\)](#) instead!

17.49.2.7 `double expLoopEnergy (int u1, int u2, int type, int type2, short si1, short sj1, short sp1, short sq1)`

Deprecated Use [exp_E_IntLoop\(\)](#) from [loop_energies.h](#) instead

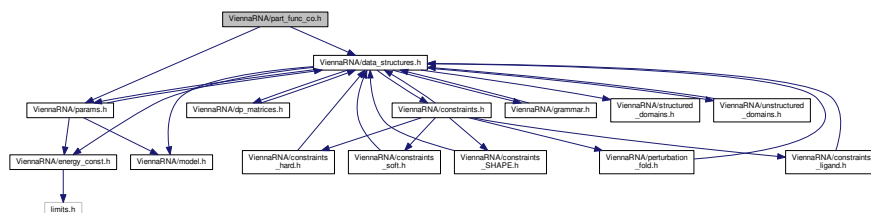
17.49.2.8 `double expHairpinEnergy (int u, int type, short si1, short sj1, const char * string)`

Deprecated Use [exp_E_Hairpin\(\)](#) from [loop_energies.h](#) instead

17.50 ViennaRNA/part_func_co.h File Reference

Partition function for two RNA sequences.

Include dependency graph for `part_func_co.h`:



Data Structures

- struct [vrna_dimer_pf_s](#)
Data structure returned by [vrna_pf_dimer\(\)](#) [More...](#)
- struct [vrna_dimer_conc_s](#)
Data structure for concentration dependency computations. [More...](#)

Typedefs

- typedef struct [vrna_dimer_pf_s](#) [vrna_dimer_pf_t](#)
Typename for the data structure that stores the dimer partition functions, [vrna_dimer_pf_s](#), as returned by [vrna_pf_dimer\(\)](#)
- typedef struct [vrna_dimer_conc_s](#) [vrna_dimer_conc_t](#)
Typename for the data structure that stores the dimer concentrations, [vrna_dimer_conc_s](#), as required by [vrna_pf_dimer_concentration\(\)](#)
- typedef struct [vrna_dimer_pf_s](#) [cofoldF](#)
Backward compatibility typedef for [vrna_dimer_pf_s](#).
- typedef struct [vrna_dimer_conc_s](#) [ConcEnt](#)
Backward compatibility typedef for [vrna_dimer_conc_s](#).

Functions

- [vrna_dimer_pf_t](#) [vrna_pf_dimer](#) ([vrna_fold_compound_t](#) *vc, char *structure)
Calculate partition function and base pair probabilities of nucleic acid/nucleic acid dimers.
- void [vrna_pf_dimer_probs](#) (double FAB, double FA, double FB, [vrna_plist_t](#) *prAB, const [vrna_plist_t](#) *prA, const [vrna_plist_t](#) *prB, int Alength, const [vrna_exp_param_t](#) *exp_params)
Compute Boltzmann probabilities of dimerization without homodimers.
- [vrna_dimer_conc_t](#) * [vrna_pf_dimer_concentrations](#) (double FcAB, double FcAA, double FcBB, double FEA, double FEB, const double *startconc, const [vrna_exp_param_t](#) *exp_params)
Given two start monomer concentrations a and b, compute the concentrations in thermodynamic equilibrium of all dimers and the monomers.
- [vrna_dimer_pf_t](#) [co_pf_fold](#) (char *sequence, char *structure)
Calculate partition function and base pair probabilities.
- [vrna_dimer_pf_t](#) [co_pf_fold_par](#) (char *sequence, char *structure, [vrna_exp_param_t](#) *parameters, int calculate_bppm, int is_constrained)
Calculate partition function and base pair probabilities.
- [vrna_plist_t](#) * [get_plist](#) ([vrna_plist_t](#) *pl, int length, double cut_off)
- void [compute_probabilities](#) (double FAB, double FEA, double FEB, [vrna_plist_t](#) *prAB, [vrna_plist_t](#) *prA, [vrna_plist_t](#) *prB, int Alength)
Compute Boltzmann probabilities of dimerization without homodimers.
- [vrna_dimer_conc_t](#) * [get_concentrations](#) (double FEAB, double FEAA, double FEBB, double FEA, double FEB, double *startconc)
Given two start monomer concentrations a and b, compute the concentrations in thermodynamic equilibrium of all dimers and the monomers.
- void [init_co_pf_fold](#) (int length)
- [FLT_OR_DBL](#) * [export_co_bppm](#) (void)
Get a pointer to the base pair probability array.
- void [free_co_pf_arrays](#) (void)
Free the memory occupied by [co_pf_fold\(\)](#)
- void [update_co_pf_params](#) (int length)
Recalculate energy parameters.
- void [update_co_pf_params_par](#) (int length, [vrna_exp_param_t](#) *parameters)
Recalculate energy parameters.

Variables

- int [mirnatog](#)
Toggles no intrabp in 2nd mol.
- double [F_monomer](#) [2]
Free energies of the two monomers.

17.50.1 Detailed Description

Partition function for two RNA sequences.

17.50.2 Function Documentation

17.50.2.1 `vrna_dimer_pf_t co_pf_fold (char * sequence, char * structure)`

Calculate partition function and base pair probabilities.

This is the cofold partition function folding. The second molecule starts at the [cut_point](#) nucleotide.

Note

OpenMP: Since this function relies on the global parameters [do_backtrack](#), [dangles](#), [temperature](#) and [pf_scale](#) it is not threadsafe according to concurrent changes in these variables! Use [co_pf_fold_par\(\)](#) instead to circumvent this issue.

Deprecated {Use [vrna_pf_dimer\(\)](#) instead!}

Parameters

<i>sequence</i>	Concatenated RNA sequences
<i>structure</i>	Will hold the structure or constraints

Returns

`vrna_dimer_pf_t` structure containing a set of energies needed for concentration computations.

17.50.2.2 `vrna_dimer_pf_t co_pf_fold_par (char * sequence, char * structure, vrna_exp_param_t * parameters, int calculate_bppm, int is_constrained)`

Calculate partition function and base pair probabilities.

This is the cofold partition function folding. The second molecule starts at the [cut_point](#) nucleotide.

Deprecated Use [vrna_pf_dimer\(\)](#) instead!

See also

[get_boltzmann_factors\(\)](#), [co_pf_fold\(\)](#)

Parameters

<i>sequence</i>	Concatenated RNA sequences
<i>structure</i>	Pointer to the structure constraint
<i>parameters</i>	Data structure containing the precalculated Boltzmann factors
<i>calculate_bppm</i>	Switch to turn Base pair probability calculations on/off (0==off) Generated by Doxygen
<i>is_constrained</i>	Switch to indicate that a structure constraint is passed via the structure argument (0==off)

Returns

vrna_dimer_pf_t structure containing a set of energies needed for concentration computations.

17.50.2.3 `vrna_plist_t* get_plist (vrna_plist_t * pl, int length, double cut_off)`

DO NOT USE THIS FUNCTION ANYMORE

Deprecated { This function is deprecated and will be removed soon!} use `assign_plist_from_pr()` instead!

17.50.2.4 `void compute_probabilities (double FAB, double FEA, double FEB, vrna_plist_t * prAB, vrna_plist_t * prA, vrna_plist_t * prB, int Alength)`

Compute Boltzmann probabilities of dimerization without homodimers.

Given the pair probabilities and free energies (in the null model) for a dimer AB and the two constituent monomers A and B, compute the conditional pair probabilities given that a dimer AB actually forms. Null model pair probabilities are given as a list as produced by `assign_plist_from_pr()`, the dimer probabilities 'prAB' are modified in place.

Deprecated { Use `vrna_pf_dimer_probs()` instead!}

Parameters

<i>FAB</i>	free energy of dimer AB
<i>FEA</i>	free energy of monomer A
<i>FEB</i>	free energy of monomer B
<i>prAB</i>	pair probabilities for dimer
<i>prA</i>	pair probabilities monomer
<i>prB</i>	pair probabilities monomer
<i>Alength</i>	Length of molecule A

17.50.2.5 `vrna_dimer_conc_t* get_concentrations (double FEAB, double FEAA, double FEBB, double FEA, double FEB, double * startconc)`

Given two start monomer concentrations a and b, compute the concentrations in thermodynamic equilibrium of all dimers and the monomers.

This function takes an array 'startconc' of input concentrations with alternating entries for the initial concentrations of molecules A and B (terminated by two zeroes), then computes the resulting equilibrium concentrations from the free energies for the dimers. Dimer free energies should be the dimer-only free energies, i.e. the FcAB entries from the `vrna_dimer_pf_t` struct.

Deprecated { Use `vrna_pf_dimer_concentrations()` instead!}

Parameters

<i>FEAB</i>	Free energy of AB dimer (FcAB entry)
<i>FEAA</i>	Free energy of AA dimer (FcAB entry)
<i>FEBB</i>	Free energy of BB dimer (FcAB entry)
<i>FEA</i>	Free energy of monomer A
<i>FEB</i>	Free energy of monomer B
<i>startconc</i>	List of start concentrations [a0],[b0],[a1],[b1],...,[an],[bn],[0],[0]

Returns

`vrna_dimer_conc_t` array containing the equilibrium energies and start concentrations

17.50.2.6 `void init_co_pf_fold (int length)`

DO NOT USE THIS FUNCTION ANYMORE

Deprecated { This function is deprecated and will be removed soon! }

17.50.2.7 `FLT_OR_DBL* export_co_bppm (void)`

Get a pointer to the base pair probability array.

Accessing the base pair probabilities for a pair (i,j) is achieved by

```
FLT_OR_DBL *pr = export_bppm(); pr_ij = pr[iindx[i]-j];
```

Deprecated This function is deprecated and will be removed soon! The base pair probability array is available through the `vrna_fold_compound_t` data structure, and its associated `vrna_mx_pf_t` member.

See also

[vrna_idx_row_wise\(\)](#)

Returns

A pointer to the base pair probability array

17.50.2.8 `void free_co_pf_arrays (void)`

Free the memory occupied by `co_pf_fold()`

Deprecated This function will be removed for the new API soon! See [vrna_pf_dimer\(\)](#), [vrna_fold_compound\(\)](#), and [vrna_fold_compound_free\(\)](#) for an alternative

17.50.2.9 `void update_co_pf_params (int length)`

Recalculate energy parameters.

This function recalculates all energy parameters given the current model settings.

Deprecated Use [vrna_exp_params_subst\(\)](#) instead!

Parameters

<i>length</i>	Length of the current RNA sequence
---------------	------------------------------------

17.50.2.10 void update_co_pf_params_par (int *length*, vrna_exp_param_t * *parameters*)

Recalculate energy parameters.

This function recalculates all energy parameters given the current model settings. It's second argument can either be NULL or a data structure containing the precomputed Boltzmann factors. In the first scenario, the necessary data structure will be created automatically according to the current global model settings, i.e. this mode might not be threadsafe. However, if the provided data structure is not NULL, threadsafety for the model parameters [dangles](#), [pf_scale](#) and [temperature](#) is regained, since their values are taken from this data structure during subsequent calculations.

Deprecated Use `vrna_exp_params_subst()` instead!

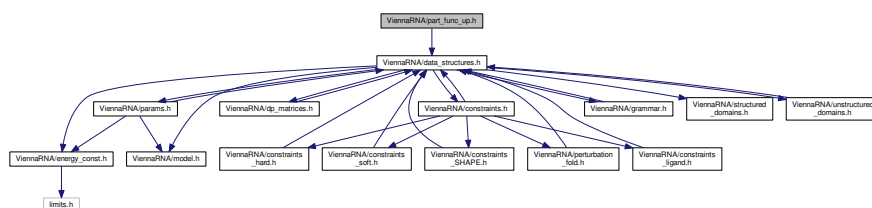
Parameters

<i>length</i>	Length of the current RNA sequence
<i>parameters</i>	data structure containing the precomputed Boltzmann factors

17.51 ViennaRNA/part_func_up.h File Reference

Implementations for accessibility and RNA-RNA interaction as a stepwise process.

Include dependency graph for `part_func_up.h`:



Functions

- `pu_contrib * pf_unstru` (char *sequence, int max_w)
Calculate the partition function over all unpaired regions of a maximal length.
- `interact * pf_interact` (const char *s1, const char *s2, `pu_contrib` *p_c, `pu_contrib` *p_c2, int max_w, char *cstruc, int incr3, int incr5)
Calculates the probability of a local interaction between two sequences.
- void `free_interact` (`interact` *pin)
Frees the output of function `pf_interact()`.
- void `free_pu_contrib_struct` (`pu_contrib` *pu)
Frees the output of function `pf_unstru()`.

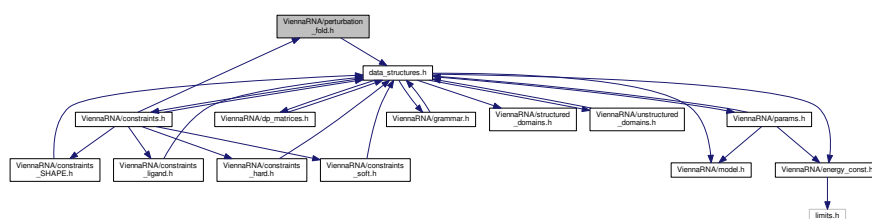
17.51.1 Detailed Description

Implementations for accessibility and RNA-RNA interaction as a stepwise process.

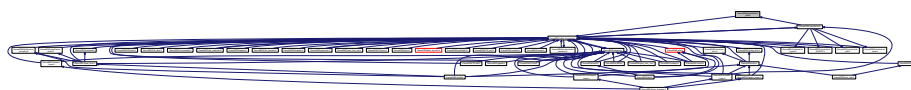
17.52 ViennaRNA/perturbation_fold.h File Reference

Find a vector of perturbation energies that minimizes the discrepancies between predicted and observed pairing probabilities and the amount of necessary adjustments.

Include dependency graph for perturbation_fold.h:



This graph shows which files directly or indirectly include this file:



Macros

- `#define VRNA_OBJECTIVE_FUNCTION_QUADRATIC 0`
Use the sum of squared aberrations as objective function.
- `#define VRNA_OBJECTIVE_FUNCTION_ABSOLUTE 1`
Use the sum of absolute aberrations as objective function.
- `#define VRNA_MINIMIZER_DEFAULT 0`
Use a custom implementation of the gradient descent algorithm to minimize the objective function.
- `#define VRNA_MINIMIZER_CONJUGATE_FR 1`
Use the GNU Scientific Library implementation of the Fletcher-Reeves conjugate gradient algorithm to minimize the objective function.
- `#define VRNA_MINIMIZER_CONJUGATE_PR 2`
Use the GNU Scientific Library implementation of the Polak-Ribiere conjugate gradient algorithm to minimize the objective function.
- `#define VRNA_MINIMIZER_VECTOR_BFGS 3`
Use the GNU Scientific Library implementation of the vector Broyden-Fletcher-Goldfarb-Shanno algorithm to minimize the objective function.
- `#define VRNA_MINIMIZER_VECTOR_BFGS2 4`
Use the GNU Scientific Library implementation of the vector Broyden-Fletcher-Goldfarb-Shanno algorithm to minimize the objective function.
- `#define VRNA_MINIMIZER_STEEPEST_DESCENT 5`
Use the GNU Scientific Library implementation of the steepest descent algorithm to minimize the objective function.

Typedefs

- typedef void(* [progress_callback](#)) (int iteration, double score, double *epsilon)
Callback for following the progress of the minimization process.

Functions

- void [vrna_sc_minimize_perturbation](#) ([vrna_fold_compound_t](#) *vc, const double *q_prob_unpaired, int objective_function, double sigma_squared, double tau_squared, int algorithm, int sample_size, double *epsilon, double initialStepSize, double minStepSize, double minImprovement, double minimizerTolerance, [progress_callback](#) callback)
Find a vector of perturbation energies that minimizes the discrepancies between predicted and observed pairing probabilities and the amount of necessary adjustments.

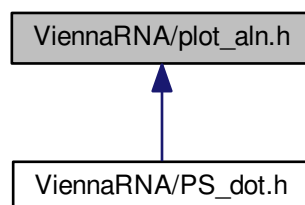
17.52.1 Detailed Description

Find a vector of perturbation energies that minimizes the discrepancies between predicted and observed pairing probabilities and the amount of necessary adjustments.

17.53 ViennaRNA/plot_aln.h File Reference

Various functions for plotting Sequence / Structure Alignments.

This graph shows which files directly or indirectly include this file:



Functions

- int [PS_color_aln](#) (const char *structure, const char *filename, const char *seqs[], const char *names[])
Produce PostScript sequence alignment color-annotated by consensus structure.
- int [aliPS_color_aln](#) (const char *structure, const char *filename, const char *seqs[], const char *names[])

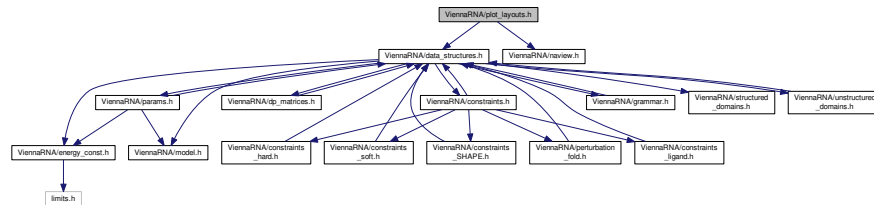
17.53.1 Detailed Description

Various functions for plotting Sequence / Structure Alignments.

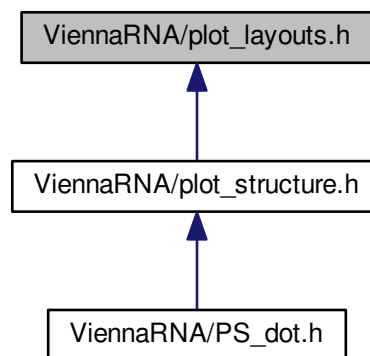
17.54 ViennaRNA/plot_layouts.h File Reference

Secondary structure plot layout algorithms.

Include dependency graph for plot_layouts.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [COORDINATE](#)
this is a workaround for the SWIG Perl Wrapper RNA plot function that returns an array of type [COORDINATE](#)
- #define [VRNA_PLOT_TYPE_SIMPLE](#) 0
Definition of Plot type simple
- #define [VRNA_PLOT_TYPE_NAVIEW](#) 1
Definition of Plot type Naview
- #define [VRNA_PLOT_TYPE_CIRCULAR](#) 2
Definition of Plot type Circular
- int [rna_plot_type](#)
Switch for changing the secondary structure layout algorithm.
- int [simple_xy_coordinates](#) (short *pair_table, float *X, float *Y)
Calculate nucleotide coordinates for secondary structure plot the Simple way
- int [simple_circplot_coordinates](#) (short *pair_table, float *x, float *y)
Calculate nucleotide coordinates for Circular Plot

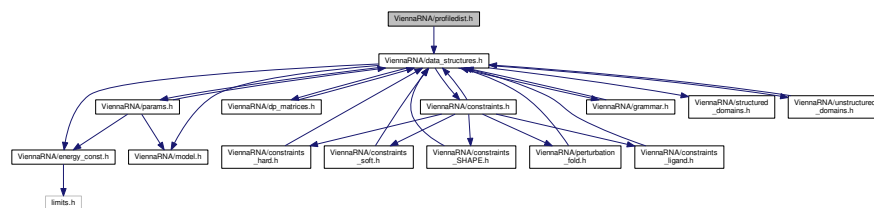
- int [xrna_plot](#) (char *string, char *structure, char *ssfile)
Produce a secondary structure plot for further editing in XRNA.
- int [PS_rna_plot](#) (char *string, char *structure, char *file)
Produce a secondary structure graph in PostScript and write it to 'filename'.
- int [PS_rna_plot_a](#) (char *string, char *structure, char *file, char *pre, char *post)
Produce a secondary structure graph in PostScript including additional annotation macros and write it to 'filename'.
- int [PS_rna_plot_a_gquad](#) (char *string, char *structure, char *ssfile, char *pre, char *post)
Produce a secondary structure graph in PostScript including additional annotation macros and write it to 'filename' (detect and draw g-quadruplexes)

17.55.1 Detailed Description

Various functions for plotting RNA secondary structures.

17.56 ViennaRNA/profiledist.h File Reference

Include dependency graph for profiledist.h:



Functions

- float [profile_edit_distance](#) (const float *T1, const float *T2)
Align the 2 probability profiles T1, T2
- float * [Make_bp_profile_bppm](#) (FLT_OR_DBL *bppm, int length)
condense pair probability matrix into a vector containing probabilities for unpaired, upstream paired and downstream paired.
- void [print_bppm](#) (const float *T)
print string representation of probability profile
- void [free_profile](#) (float *T)
free space allocated in Make_bp_profile
- float * [Make_bp_profile](#) (int length)

17.56.1 Function Documentation

17.56.1.1 float profile_edit_distance (const float * T1, const float * T2)

Align the 2 probability profiles T1, T2

.

This is like a Needleman-Wunsch alignment, we should really use affine gap-costs ala Gotoh


```
17.56.1.2 float* Make_bp_profile_bppm ( FLT_OR_DBL * bppm, int length )
```

condense pair probability matrix into a vector containing probabilities for unpaired, upstream paired and downstream paired.

This resulting probability profile is used as input for `profile_edit_distance`

Parameters

<i>bppm</i>	A pointer to the base pair probability matrix
<i>length</i>	The length of the sequence

Returns

The bp profile

17.56.1.3 void free_profile (float * *T*)

free space allocated in Make_bp_profile

Backward compatibility only. You can just use plain `free()`

17.56.1.4 float* Make_bp_profile (int *length*)

Note

This function is NOT threadsafe

See also

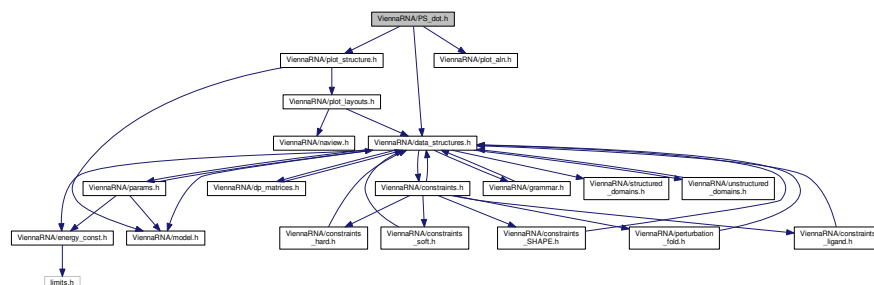
Make_bp_profile_bpppm()

Deprecated This function is deprecated and will be removed soon! See [Make_bp_profile_bppm\(\)](#) for a replacement

17.57 ViennaRNA/PS_dot.h File Reference

Various functions for plotting RNA secondary structures, dot-plots and other visualizations.

Include dependency graph for PS_dot.h:



Data Structures

- struct [vrna_dotplot_auxdata_t](#)
- int [PS_dot_plot_list](#) (char *seq, char *filename, [plist](#) *pl, [plist](#) *mf, char *comment)
Produce a postscript dot-plot from two pair lists.
- int [PS_dot_plot](#) (char *string, char *file)
Produce postscript dot-plot.

17.57.1 Detailed Description

Various functions for plotting RNA secondary structures, dot-plots and other visualizations.

17.58 ViennaRNA/read_epars.h File Reference

Read and write energy parameter files.

Functions

- void [read_parameter_file](#) (const char fname[])
Read energy parameters from a file.
- void [write_parameter_file](#) (const char fname[])
Write energy parameters to a file.

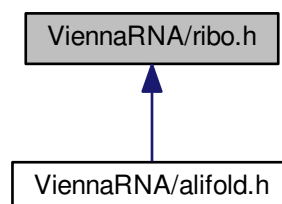
17.58.1 Detailed Description

Read and write energy parameter files.

17.59 ViennaRNA/ribo.h File Reference

Parse RiboSum Scoring Matrices for Covariance Scoring of Alignments.

This graph shows which files directly or indirectly include this file:



Functions

- float ** [get_ribosum](#) (const char **Alseq, int n_seq, int length)
Retrieve a RiboSum Scoring Matrix for a given Alignment.
- float ** [readribosum](#) (char *name)
Read a RiboSum or other user-defined Scoring Matrix and Store into global Memory.

17.59.1 Detailed Description

Parse RiboSum Scoring Matrices for Covariance Scoring of Alignments.

17.60 ViennaRNA/RNAstruct.h File Reference

Parsing and Coarse Graining of Structures.

Functions

- char * [b2HIT](#) (const char *structure)
Converts the full structure from bracket notation to the HIT notation including root.
- char * [b2C](#) (const char *structure)
Converts the full structure from bracket notation to the a coarse grained notation using the 'H' 'B' 'I' 'M' and 'R' identifiers.
- char * [b2Shapiro](#) (const char *structure)
Converts the full structure from bracket notation to the weighted coarse grained notation using the 'H' 'B' 'I' 'M' 'S' 'E' and 'R' identifiers.
- char * [add_root](#) (const char *structure)
Adds a root to an un-rooted tree in any except bracket notation.
- char * [expand_Shapiro](#) (const char *coarse)
Inserts missing 'S' identifiers in unweighted coarse grained structures as obtained from [b2C\(\)](#).
- char * [expand_Full](#) (const char *structure)
Convert the full structure from bracket notation to the expanded notation including root.
- char * [unexpand_Full](#) (const char *ffull)
Restores the bracket notation from an expanded full or HIT tree, that is any tree using only identifiers 'U' 'P' and 'R'.
- char * [unweight](#) (const char *wcoarse)
Strip weights from any weighted tree.
- void [unexpand_aligned_F](#) (char *align[2])
Converts two aligned structures in expanded notation.
- void [parse_structure](#) (const char *structure)
Collects a statistic of structure elements of the full structure in bracket notation.

Variables

- int `loop_size` [STRUC]
contains a list of all loop sizes. `loop_size[0]` contains the number of external bases.
- int `helix_size` [STRUC]
contains a list of all stack sizes.
- int `loop_degree` [STRUC]
contains the corresponding list of loop degrees.
- int `loops`
contains the number of loops (and therefore of stacks).
- int `unpaired`
contains the number of unpaired bases.
- int `pairs`
contains the number of base pairs in the last parsed structure.

17.60.1 Detailed Description

Parsing and Coarse Graining of Structures.

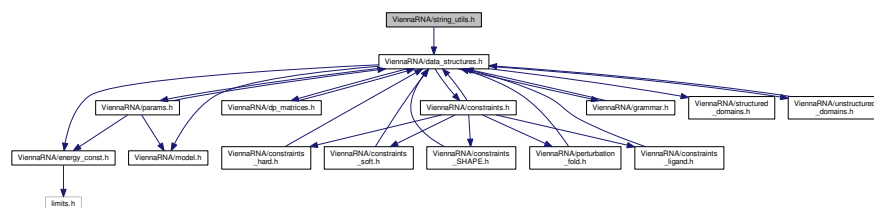
Example:

```
* .(((.....))..((.....))). is the bracket or full tree
* becomes expanded: - expand_Full() -
* ((U)((U)(U)((U)(U)(U)P)P)(U)(U)((U)(U)P)P)P)(U)R)
* HIT: - b2HIT() -
* ((U1)((U2)((U3)P3)(U2)((U2)P2)P2)(U1)R)
* Coarse: - b2C() -
* ((H)((H)M)R)
* becomes expanded: - expand_Shapiro() -
* (((((H)S)((H)S)M)S)R)
* weighted Shapiro: - b2Shapiro() -
* (((((H3)S3)((H2)S2)M4)S2)E2)R)
*
```

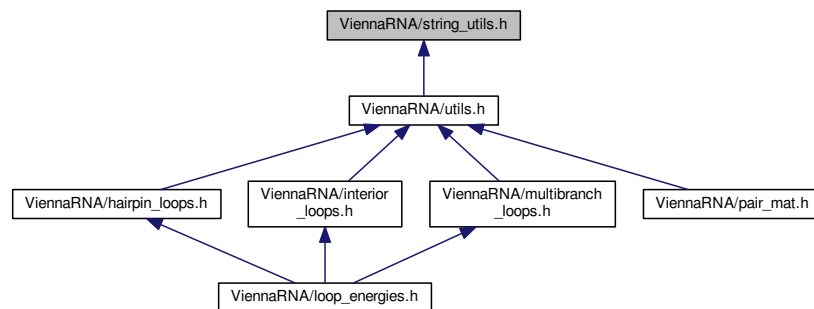
17.61 ViennaRNA/string_utils.h File Reference

General utility- and helper-functions for RNA sequence and structure strings used throughout the ViennaRNA Package.

Include dependency graph for `string_utils.h`:



This graph shows which files directly or indirectly include this file:



Functions

- void [str_uppercase](#) (char *sequence)
Convert an input sequence to uppercase.
- void [str_DNA2RNA](#) (char *sequence)
Convert a DNA input sequence to RNA alphabet.
- char * [random_string](#) (int l, const char symbols[])
Create a random string using characters from a specified symbol set.
- int [hamming](#) (const char *s1, const char *s2)
Calculate hamming distance between two sequences.
- int [hamming_bound](#) (const char *s1, const char *s2, int n)
Calculate hamming distance between two sequences up to a specified length.

- #define [XSTR](#)(s) [STR](#)(s)
Stringify a macro after expansion.
- #define [STR](#)(s) #s
Stringify a macro argument.
- #define [FILENAME_MAX_LENGTH](#) 80
Maximum length of filenames that are generated by our programs.
- #define [FILENAME_ID_LENGTH](#) 42
Maximum length of id taken from fasta header for filename generation.
- char * [vrna_strdup_printf](#) (const char *format,...)
Safely create a formatted string.
- char * [vrna_strdup_vprintf](#) (const char *format, va_list argp)
Safely create a formatted string.
- int [vrna_strcat_printf](#) (char **dest, const char *format,...)
Safely append a formatted string to another string.
- int [vrna_strcat_vprintf](#) (char **dest, const char *format, va_list args)
Safely append a formatted string to another string.
- char * [vrna_random_string](#) (int l, const char symbols[])
Create a random string using characters from a specified symbol set.
- int [vrna_hamming_distance](#) (const char *s1, const char *s2)
Calculate hamming distance between two sequences.
- int [vrna_hamming_distance_bound](#) (const char *s1, const char *s2, int n)

Calculate hamming distance between two sequences up to a specified length.

- void [vrna_seq_toRNA](#) (char *sequence)

Convert an input sequence (possibly containing DNA alphabet characters) to RNA alphabet.

- void [vrna_seq_toupper](#) (char *sequence)

Convert an input sequence to uppercase.

- char * [vrna_cut_point_insert](#) (const char *string, int cp)

Add a separating '&' character into a string according to cut-point position.

- char * [vrna_cut_point_remove](#) (const char *string, int *cp)

Remove a separating '&' character from a string.

17.61.1 Detailed Description

General utility- and helper-functions for RNA sequence and structure strings used throughout the ViennaRNA Package.

17.61.2 Function Documentation

17.61.2.1 void str_uppercase (char * sequence)

Convert an input sequence to uppercase.

Deprecated Use [vrna_seq_toupper\(\)](#) instead!

17.61.2.2 void str_DNA2RNA (char * sequence)

Convert a DNA input sequence to RNA alphabet.

Deprecated Use [vrna_seq_toRNA\(\)](#) instead!

17.61.2.3 char* random_string (int l, const char symbols[])

Create a random string using characters from a specified symbol set.

Deprecated Use [vrna_random_string\(\)](#) instead!

17.61.2.4 int hamming (const char * s1, const char * s2)

Calculate hamming distance between two sequences.

Deprecated Use [vrna_hamming_distance\(\)](#) instead!

17.61.2.5 `int hamming_bound (const char * s1, const char * s2, int n)`

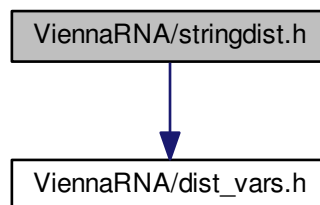
Calculate hamming distance between two sequences up to a specified length.

Deprecated Use `vrna_hamming_distance_bound()` instead!

17.62 ViennaRNA/stringdist.h File Reference

Functions for String Alignment.

Include dependency graph for stringdist.h:



Functions

- `swString * Make_swString (char *string)`
Convert a structure into a format suitable for `string_edit_distance()`.
- `float string_edit_distance (swString *T1, swString *T2)`
Calculate the string edit distance of T1 and T2.

17.62.1 Detailed Description

Functions for String Alignment.

17.62.2 Function Documentation

17.62.2.1 `swString* Make_swString (char * string)`

Convert a structure into a format suitable for `string_edit_distance()`.

Parameters

<code>string</code>	
---------------------	--

Data Structures

- struct [vrna_hx_s](#)
Data structure representing an entry of a helix list.
- typedef struct [vrna_hx_s](#) [vrna_hx_t](#)
Convenience typedef for data structure [vrna_hx_s](#).
- char * [vrna_db_pack](#) (const char *struc)
Pack secondary secondary structure, 5:1 compression using base 3 encoding.
- char * [vrna_db_unpack](#) (const char *packed)
Unpack secondary structure previously packed with [vrna_db_pack\(\)](#)
- short * [vrna_ptable](#) (const char *structure)
Create a pair table of a secondary structure.
- short * [vrna_pt_pk_get](#) (const char *structure)
Create a pair table of a secondary structure (pseudo-knot version)
- short * [vrna_ptable_copy](#) (const short *pt)
Get an exact copy of a pair table.
- short * [vrna_pt_ali_get](#) (const char *structure)
Create a pair table of a secondary structure (snoop align version)
- short * [vrna_pt_snoop_get](#) (const char *structure)
Create a pair table of a secondary structure (snoop version)
- int * [vrna_loopidx_from_ptable](#) (const short *pt)
Get a loop index representation of a structure.
- char * [vrna_db_from_ptable](#) (short *pt)
Convert a pair table into dot-parenthesis notation.
- int [vrna_bp_distance](#) (const char *str1, const char *str2)
Compute the "base pair" distance between two secondary structures s1 and s2.
- unsigned int * [vrna_refBPcnt_matrix](#) (const short *reference_pt, unsigned int turn)
Make a reference base pair count matrix.
- unsigned int * [vrna_refBPdist_matrix](#) (const short *pt1, const short *pt2, unsigned int turn)
Make a reference base pair distance matrix.
- char * [vrna_db_from_probs](#) (const FLT_OR_DBL *pr, unsigned int length)
Create a dot-bracket like structure string from base pair probability matrix.
- char [vrna_bpp_symbol](#) (const float *x)
Get a pseudo dot bracket notation for a given probability information.
- char * [vrna_db_from_bp_stack](#) ([vrna_bp_stack_t](#) *bp, unsigned int length)
Create a dot-bracket/parenthesis structure from backtracking stack.
- [vrna_plist_t](#) * [vrna_plist](#) (const char *struc, float pr)
Create a [vrna_plist_t](#) from a dot-bracket string.
- [vrna_plist_t](#) * [vrna_plist_from_probs](#) ([vrna_fold_compound_t](#) *vc, double cut_off)
Create a [vrna_plist_t](#) from base pair probability matrix.
- char * [vrna_db_from_plist](#) ([vrna_plist_t](#) *pairs, unsigned int n)
Convert a list of base pairs into dot-bracket notation.
- void [assign_plist_from_db](#) ([vrna_plist_t](#) **pl, const char *struc, float pr)
Create a [vrna_plist_t](#) from a dot-bracket string.
- char * [pack_structure](#) (const char *struc)
Pack secondary secondary structure, 5:1 compression using base 3 encoding.
- char * [unpack_structure](#) (const char *packed)
Unpack secondary structure previously packed with [pack_structure\(\)](#)
- short * [make_pair_table](#) (const char *structure)

Create a pair table of a secondary structure.

- short * [copy_pair_table](#) (const short *pt)

Get an exact copy of a pair table.

- short * [alimake_pair_table](#) (const char *structure)
- short * [make_pair_table_snoop](#) (const char *structure)
- int [bp_distance](#) (const char *str1, const char *str2)

Compute the "base pair" distance between two secondary structures s1 and s2.

- unsigned int * [make_referenceBP_array](#) (short *reference_pt, unsigned int turn)

Make a reference base pair count matrix.

- unsigned int * [compute_BPdifferences](#) (short *pt1, short *pt2, unsigned int turn)

Make a reference base pair distance matrix.

- void [assign_plist_from_pr](#) (vrna_plist_t **pl, FLT_OR_DBL *probs, int length, double cutoff)

Create a vrna_plist_t from a probability matrix.

- void [parenthesis_structure](#) (char *structure, vrna_bp_stack_t *bp, int length)

Create a dot-bracket/parenthesis structure from backtracking stack.

- void [parenthesis_zuker](#) (char *structure, vrna_bp_stack_t *bp, int length)

Create a dot-bracket/parenthesis structure from backtracking stack obtained by zuker suboptimal calculation in cofold.c.

- void [bppm_to_structure](#) (char *structure, FLT_OR_DBL *pr, unsigned int length)

Create a dot-bracket like structure string from base pair probability matrix.

- char [bppm_symbol](#) (const float *x)

Get a pseudo dot bracket notation for a given probability information.

17.63.1 Detailed Description

Various utility- and helper-functions for secondary structure parsing, converting, etc.

17.64 ViennaRNA/structured_domains.h File Reference

This module provides interfaces that deal with additional structured domains in the folding grammar.

This graph shows which files directly or indirectly include this file:



Data Structures

- struct [vrna_structured_domains_s](#)

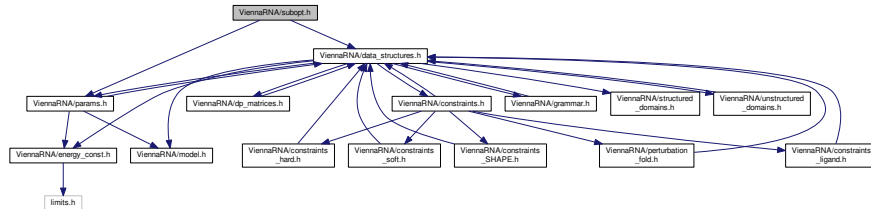
17.64.1 Detailed Description

This module provides interfaces that deal with additional structured domains in the folding grammar.

17.65 ViennaRNA/subopt.h File Reference

RNAsubopt and density of states declarations.

Include dependency graph for subopt.h:



Data Structures

- struct [vrna_subopt_sol_s](#)
Solution element from subopt.c.

Macros

- `#define` [MAXDOS](#) 1000
Maximum density of states discretization for subopt.

Typedefs

- typedef struct [vrna_subopt_sol_s](#) [vrna_subopt_solution_t](#)
Typename for the subopt solution list representing data structure [vrna_subopt_sol_s](#).
- typedef void([vrna_subopt_callback](#)) (const char *structure, float energy, void *data)
Callback for [vrna_subopt_cb\(\)](#)
- typedef struct [vrna_subopt_sol_s](#) [SOLUTION](#)
Backward compatibility typedef for [vrna_subopt_sol_s](#).

Functions

- [vrna_subopt_solution_t](#) * [vrna_subopt](#) ([vrna_fold_compound_t](#) *vc, int delta, int sorted, FILE *fp)
Returns list of subopt structures or writes to fp.
- void [vrna_subopt_cb](#) ([vrna_fold_compound_t](#) *vc, int delta, [vrna_subopt_callback](#) *cb, void *data)
Generate suboptimal structures within an energy band around the MFE.
- [vrna_subopt_solution_t](#) * [vrna_subopt_zuker](#) ([vrna_fold_compound_t](#) *vc)
Compute Zuker type suboptimal structures.
- [SOLUTION](#) * [subopt](#) (char *seq, char *structure, int delta, FILE *fp)
Returns list of subopt structures or writes to fp.
- [SOLUTION](#) * [subopt_par](#) (char *seq, char *structure, [vrna_param_t](#) *parameters, int delta, int is_↔ constrained, int is_circular, FILE *fp)
Returns list of subopt structures or writes to fp.
- [SOLUTION](#) * [subopt_circ](#) (char *seq, char *sequence, int delta, FILE *fp)
Returns list of circular subopt structures or writes to fp.
- [SOLUTION](#) * [zukersubopt](#) (const char *string)
Compute Zuker type suboptimal structures.
- [SOLUTION](#) * [zukersubopt_par](#) (const char *string, [vrna_param_t](#) *parameters)
Compute Zuker type suboptimal structures.

Variables

- double [print_energy](#)
printing threshold for use with logML
- int [subopt_sorted](#)
Sort output by energy.
- int [density_of_states](#) [MAXDOS+1]
The Density of States.

17.65.1 Detailed Description

RNAsubopt and density of states declarations.

17.65.2 Typedef Documentation

17.65.2.1 typedef struct vrna_subopt_sol_s SOLUTION

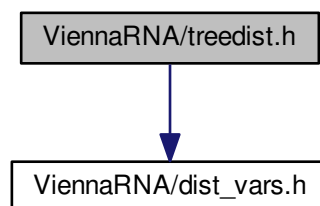
Backward compatibility typedef for [vrna_subopt_sol_s](#).

Deprecated Use [vrna_subopt_solution_t](#) instead!

17.66 ViennaRNA/treedist.h File Reference

Functions for [Tree](#) Edit Distances.

Include dependency graph for treedist.h:



Functions

- [Tree](#) * [make_tree](#) (char *struc)
Constructs a [Tree](#) (essentially the postorder list) of the structure 'struc', for use in [tree_edit_distance](#)().
- float [tree_edit_distance](#) ([Tree](#) *T1, [Tree](#) *T2)
Calculates the edit distance of the two trees.
- void [print_tree](#) ([Tree](#) *t)
Print a tree (mainly for debugging)
- void [free_tree](#) ([Tree](#) *t)
Free the memory allocated for [Tree](#) t.

17.66.1 Detailed Description

Functions for [Tree](#) Edit Distances.

17.66.2 Function Documentation

17.66.2.1 `Tree* make_tree (char * struc)`

Constructs a [Tree](#) (essentially the postorder list) of the structure 'struc', for use in [tree_edit_distance\(\)](#).

Parameters

<i>struc</i>	may be any rooted structure representation.
--------------	---------------------------------------------

Returns

17.66.2.2 `float tree_edit_distance (Tree * T1, Tree * T2)`

Calculates the edit distance of the two trees.

Parameters

<i>T1</i>	
<i>T2</i>	

Returns

17.66.2.3 `void free_tree (Tree * t)`

Free the memory allocated for [Tree](#) *t*.

Parameters

<i>t</i>	
----------	--

17.67 ViennaRNA/units.h File Reference

Physical Units and Functions to convert them into each other.

- double [vrna_convert_energy](#) (double energy, [vrna_unit_energy_e](#) from, [vrna_unit_energy_e](#) to)
Convert between energy / work units.
- double [vrna_convert_temperature](#) (double temp, [vrna_unit_temperature_e](#) from, [vrna_unit_temperature_e](#) to)
Convert between temperature units.

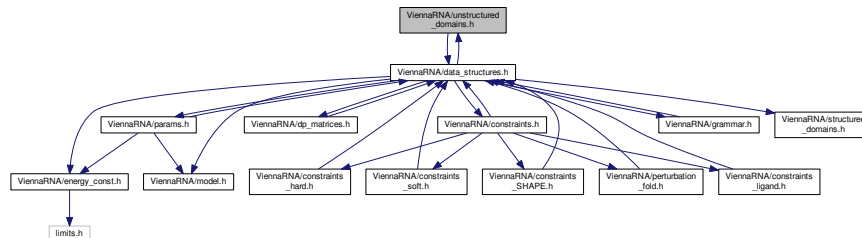
17.67.1 Detailed Description

Physical Units and Functions to convert them into each other.

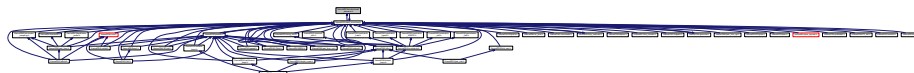
17.68 ViennaRNA/unstructured_domains.h File Reference

Functions to modify unstructured domains, e.g. to incorporate ligands binding to unpaired stretches.

Include dependency graph for unstructured_domains.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [vrna_unstructured_domain_s](#)
Data structure to store all functionality for ligand binding. [More...](#)
- struct [vrna_unstructured_domain_motif_s](#)

Macros

- `#define VRNA_UNSTRUCTURED_DOMAIN_EXT_LOOP 1U`
Flag to indicate ligand bound to unpaired stretch in the exterior loop.
- `#define VRNA_UNSTRUCTURED_DOMAIN_HP_LOOP 2U`
Flag to indicate ligand bound to unpaired stretch in a hairpin loop.
- `#define VRNA_UNSTRUCTURED_DOMAIN_INT_LOOP 4U`
Flag to indicate ligand bound to unpaired stretch in an interior loop.
- `#define VRNA_UNSTRUCTURED_DOMAIN_MB_LOOP 8U`
Flag to indicate ligand bound to unpaired stretch in a multibranch loop.
- `#define VRNA_UNSTRUCTURED_DOMAIN_MOTIF 16U`
Flag to indicate ligand binding without additional unbound nucleotides (motif-only)
- `#define VRNA_UNSTRUCTURED_DOMAIN_ALL_LOOPS (VRNA_UNSTRUCTURED_DOMAIN_EXT_LOOP | VRNA_UNSTRUCTURED_DOMAIN_HP_LOOP | VRNA_UNSTRUCTURED_DOMAIN_INT_LOOP | VRNA_UNSTRUCTURED_DOMAIN_MB_LOOP)`
Flag to indicate ligand bound to unpaired stretch in any loop (convenience macro)

Typedefs

- `typedef struct vrna_unstructured_domain_s vrna_ud_t`
Typename for the ligand binding extension data structure `vrna_unstructured_domain_s`.
- `typedef int(vrna_callback_ud_energy) (vrna_fold_compound_t *vc, int i, int j, unsigned int loop_type, void *data)`
Callback to retrieve binding free energy of a ligand bound to an unpaired sequence segment.
- `typedef FLT_OR_DBL(vrna_callback_ud_exp_energy) (vrna_fold_compound_t *vc, int i, int j, unsigned int loop_type, void *data)`
Callback to retrieve Boltzmann factor of the binding free energy of a ligand bound to an unpaired sequence segment.
- `typedef void(vrna_callback_ud_production) (vrna_fold_compound_t *vc, void *data)`
Callback for pre-processing the production rule of the ligand binding to unpaired stretches feature.
- `typedef void(vrna_callback_ud_exp_production) (vrna_fold_compound_t *vc, void *data)`
Callback for pre-processing the production rule of the ligand binding to unpaired stretches feature (partition function variant)
- `typedef void(vrna_callback_ud_probs_add) (vrna_fold_compound_t *vc, int i, int j, unsigned int loop_type, FLT_OR_DBL exp_energy, void *data)`
Callback to store/add equilibrium probability for a ligand bound to an unpaired sequence segment.
- `typedef FLT_OR_DBL(vrna_callback_ud_probs_get) (vrna_fold_compound_t *vc, int i, int j, unsigned int loop_type, int motif, void *data)`
Callback to retrieve equilibrium probability for a ligand bound to an unpaired sequence segment.

Functions

- `void vrna_ud_add_motif (vrna_fold_compound_t *vc, const char *motif, double motif_en, unsigned int loop_type)`
Add an unstructured domain motif, e.g. for ligand binding.
- `int * vrna_ud_get_motif_size_at (vrna_fold_compound_t *vc, int i, unsigned int loop_type)`
Get a list of unique motif sizes that start at a certain position within the sequence.
- `void vrna_ud_remove (vrna_fold_compound_t *vc)`
Remove ligand binding to unpaired stretches.
- `void vrna_ud_set_data (vrna_fold_compound_t *vc, void *data, vrna_callback_free_auxdata *free_cb)`
Attach an auxiliary data structure.

- void `vrna_ud_set_prod_rule_cb` (`vrna_fold_compound_t` *vc, `vrna_callback_ud_production` *pre_cb, `vrna_callback_ud_energy` *e_cb)
Attach production rule callbacks for free energies computations.
- void `vrna_ud_set_exp_prod_rule_cb` (`vrna_fold_compound_t` *vc, `vrna_callback_ud_exp_production` *pre_cb, `vrna_callback_ud_exp_energy` *exp_e_cb)
Attach production rule for partition function.
- void `vrna_ud_set_prob_cb` (`vrna_fold_compound_t` *vc, `vrna_callback_ud_probs_add` *setter, `vrna_callback_ud_probs_get` *getter)

17.68.1 Detailed Description

Functions to modify unstructured domains, e.g. to incorporate ligands binding to unpaired stretches.

17.68.2 Function Documentation

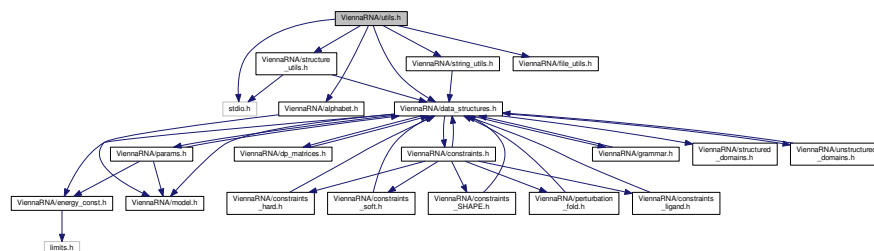
- 17.68.2.1 void `vrna_ud_set_prob_cb` (`vrna_fold_compound_t` * vc, `vrna_callback_ud_probs_add` * setter, `vrna_callback_ud_probs_get` * getter)

SWIG Wrapper Notes This function is attached as method `ud_set_prob_cb()` to objects of type `fold_compound`

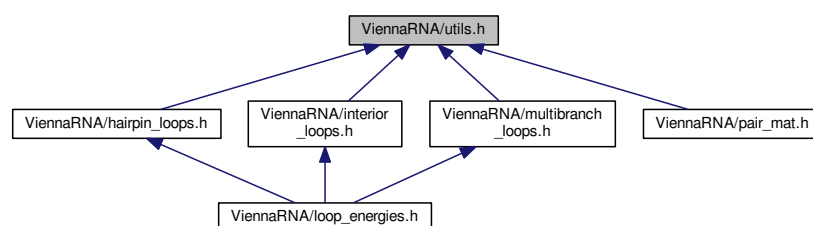
17.69 ViennaRNA/utils.h File Reference

General utility- and helper-functions used throughout the *ViennaRNA Package*.

Include dependency graph for `utils.h`:



This graph shows which files directly or indirectly include this file:



Functions

- char * [get_line](#) (FILE *fp)
Read a line of arbitrary length from a stream.
- void [print_tty_input_seq](#) (void)
Print a line to stdout that asks for an input sequence.
- void [print_tty_input_seq_str](#) (const char *s)
Print a line with a user defined string and a ruler to stdout.
- void [warn_user](#) (const char message[])
Print a warning message.
- void [nrerror](#) (const char message[])
Die with an error message.
- void * [space](#) (unsigned size)
Allocate space safely.
- void * [xrealloc](#) (void *p, unsigned size)
Reallocate space safely.
- void [init_rand](#) (void)
Make random number seeds.
- double [urn](#) (void)
get a random number from [0..1]
- int [int_urn](#) (int from, int to)
Generates a pseudo random integer in a specified range.
- void [filecopy](#) (FILE *from, FILE *to)
Inefficient `cp`
- char * [time_stamp](#) (void)
Get a timestamp.

- #define [VRNA_INPUT_ERROR](#) 1U
Output flag of [get_input_line\(\)](#): "An ERROR has occurred, maybe EOF".
- #define [VRNA_INPUT_QUIT](#) 2U
Output flag of [get_input_line\(\)](#): "the user requested quitting the program".
- #define [VRNA_INPUT_MISC](#) 4U
Output flag of [get_input_line\(\)](#): "something was read".
- #define [VRNA_INPUT_FASTA_HEADER](#) 8U
*Input/Output flag of [get_input_line\(\)](#):
if used as input option this tells [get_input_line\(\)](#) that the data to be read should comply with the FASTA format.*
- #define [VRNA_INPUT_CONSTRAINT](#) 32U
*Input flag for [get_input_line\(\)](#):
Tell [get_input_line\(\)](#) that we assume to read a structure constraint.*
- #define [VRNA_INPUT_NO_TRUNCATION](#) 256U
Input switch for [get_input_line\(\)](#): "do not truncate the line by eliminating white spaces at end of line".
- #define [VRNA_INPUT_NO_REST](#) 512U
Input switch for [vrna_file_fasta_read_record\(\)](#): "do fill rest array".
- #define [VRNA_INPUT_NO_SPAN](#) 1024U
Input switch for [vrna_file_fasta_read_record\(\)](#): "never allow data to span more than one line".
- #define [VRNA_INPUT_NOSKIP_BLANK_LINES](#) 2048U
Input switch for [vrna_file_fasta_read_record\(\)](#): "do not skip empty lines".
- #define [VRNA_INPUT_BLANK_LINE](#) 4096U
Output flag for [vrna_file_fasta_read_record\(\)](#): "read an empty line".
- #define [VRNA_INPUT_NOSKIP_COMMENTS](#) 128U
Input switch for [get_input_line\(\)](#): "do not skip comment lines".

- `#define VRNA_INPUT_COMMENT 8192U`
Output flag for `vrna_file_fasta_read_record()`: "read a comment".
- `#define MIN2(A, B) ((A) < (B) ? (A) : (B))`
Get the minimum of two comparable values.
- `#define MAX2(A, B) ((A) > (B) ? (A) : (B))`
Get the maximum of two comparable values.
- `#define MIN3(A, B, C) (MIN2(MIN2((A),(B))),(C))`
Get the minimum of three comparable values.
- `#define MAX3(A, B, C) (MAX2(MAX2((A),(B))),(C))`
Get the maximum of three comparable values.
- `unsigned short xsubi [3]`
Current 48 bit random number.
- `void * vrna_alloc (unsigned size)`
Allocate space safely.
- `void * vrna_realloc (void *p, unsigned size)`
Reallocate space safely.
- `void vrna_message_error (const char *format,...)`
Print an error message and die.
- `void vrna_message_verror (const char *format, va_list args)`
Print an error message and die.
- `void vrna_message_warning (const char *format,...)`
Print a warning message.
- `void vrna_message_vwarning (const char *format, va_list args)`
Print a warning message.
- `void vrna_message_info (FILE *fp, const char *format,...)`
Print an info message.
- `void vrna_message_vinfo (FILE *fp, const char *format, va_list args)`
Print an info message.
- `void vrna_init_rand (void)`
Initialize seed for random number generator.
- `double vrna_urn (void)`
get a random number from [0..1]
- `int vrna_int_urn (int from, int to)`
Generates a pseudo random integer in a specified range.
- `char * vrna_time_stamp (void)`
Get a timestamp.
- `unsigned int get_input_line (char **string, unsigned int options)`
- `void vrna_message_input_seq_simple (void)`
Print a line to stdout that asks for an input sequence.
- `void vrna_message_input_seq (const char *s)`
Print a line with a user defined string and a ruler to stdout.
- `int * vrna_idx_row_wise (unsigned int length)`
Get an index mapper array (iidx) for accessing the energy matrices, e.g. in partition function related functions.
- `int * vrna_idx_col_wise (unsigned int length)`
Get an index mapper array (idx) for accessing the energy matrices, e.g. in MFE related functions.

17.69.1 Detailed Description

General utility- and helper-functions used throughout the *ViennaRNA Package*.

17.69.2 Function Documentation

17.69.2.1 `char* get_line (FILE * fp)`

Read a line of arbitrary length from a stream.

Returns a pointer to the resulting string. The necessary memory is allocated and should be released using `free()` when the string is no longer needed.

Deprecated Use `vrna_read_line()` as a substitute!

Parameters

<i>fp</i>	A file pointer to the stream where the function should read from
-----------	------------------------------------------------------------------

Returns

A pointer to the resulting string

17.69.2.2 `void print_tty_input_seq (void)`

Print a line to `stdout` that asks for an input sequence.

There will also be a ruler (scale line) printed that helps orientation of the sequence positions

Deprecated Use `vrna_message_input_seq_simple()` instead!

17.69.2.3 `void print_tty_input_seq_str (const char * s)`

Print a line with a user defined string and a ruler to `stdout`.

(usually this is used to ask for user input) There will also be a ruler (scale line) printed that helps orientation of the sequence positions

Deprecated Use `vrna_message_input_seq()` instead!

17.69.2.4 `void warn_user (const char message[])`

Print a warning message.

Print a warning message to `stderr`

Deprecated Use `vrna_message_warning()` instead!

17.69.2.5 `void nerror (const char message[])`

Die with an error message.

Deprecated Use `vrna_message_error()` instead!

17.69.2.6 `void* space (unsigned size)`

Allocate space safely.

Deprecated Use `vrna_alloc()` instead!

17.69.2.7 `void* xrealloc (void * p, unsigned size)`

Reallocate space safely.

Deprecated Use `vrna_realloc()` instead!

17.69.2.8 `void init_rand (void)`

Make random number seeds.

Deprecated Use `vrna_init_rand()` instead!

17.69.2.9 `double urn (void)`

get a random number from [0..1]

Deprecated Use `vrna_urn()` instead!

17.69.2.10 `int int_urn (int from, int to)`

Generates a pseudo random integer in a specified range.

Deprecated Use `vrna_int_urn()` instead!

17.69.2.11 `void filecopy (FILE * from, FILE * to)`

Inefficient `cp`

Deprecated Use `vrna_file_copy()` instead!

17.69.2.12 `char* time_stamp (void)`

Get a timestamp.

Deprecated Use `vrna_time_stamp()` instead!

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