mm_trj2pdb

V.1.0.2

Generated by Doxygen 1.8.5

Fri Aug 30 2013 03:08:59

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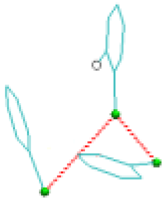
mm_trj2pdb



1.1 Introduction

About this program:

- Program that creates PDB file from trajectory snapshot

Developer:

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License:

- GPL

1.2 How to use

Usage:

```
mm_trj2pdb -i INPUT -o OUTPUT [ -l LOGFILE ] [ -q ] [ -h ]

Parametrs:
   -i          - input file name
   -o          - output file name
   -l          - log enable
   -q          - quiet enable
   -h          - show this help and exit
```

Chapter 2

Install

2.1 Requirements

The application mm_trj2pdb requires the following external stuff:

- cmake >= 2.8
- gcc >= 4.8

2.2 How to install

2.2.1 Linux

```
* mkdir build && cd build
* cmake -DCMAKE_INSTALL_PREFIX=/usr -DCMAKE_BUILD_TYPE=Release ../
* make
* make install
*
```

2.2.2 Windows

```
* create project file using 'cmake'
* compile project
*
```

You may also download compiled executable file for Win_x86.

Chapter 3

Changelog

V.1.0.2 (2013-07-27)

- initial release

Chapter 4

File Index

4.1 File List

Here is a list of all files with brief descriptions:

Chapter 5

File Documentation

5.1 src/add_main.c File Reference

```
#include <stdio.h>
#include "messages.h"
```

Functions

- int error_checking (const const char ∗input, const char ∗output)

  function that checks errors in input variables
- int print_message (const int quiet, FILE ∗std_output, const int log, FILE ∗f_log, const int mode, const char ∗str)

  function that prints message in log and stdout
- int set_defaults (char ∗input, int ∗log, char ∗output, int ∗quiet)

  function that sets default values of variables

5.1.1 Function Documentation

5.1.1.1 int error_checking (const const char ∗ *input,* const char ∗ *output*)

function that checks errors in input variables

```
* error_checking (input, output);
*
```

Parameters

aglinp	aglomerate file name
cell	massive of cell size
input	input file name
output	output file name

Returns

11 - error in ’input’
12 - error in ’output’
0 - exit without errors

5.1.1.2 int print_message (const int *quiet,* FILE ∗ *std_output,* const int *log,* FILE ∗ *f_log,* const int *mode,* const char ∗ *str*)

function that prints message in log and stdout

```
* print_message (quiet, stdout, log, f_log, 0, str);
*
```

Parameters

quiet	status of quiet-mode
std_output	stdout
log	status of log-mode
f_log	log file
mode	number of message in "messages.c"
str	additional text in message

Returns

0 - exit without errors

5.1.1.3 int set_defaults (char ∗ *input,* int ∗ *log,* char ∗ *output,* int ∗ *quiet*)

function that sets default values of variables

```
* set_defaults (input, &log, output, &quiet);
*
```

Parameters

input	mask of trajectory files
log	status of log-mode
output	output file name
quiet	status of quiet-mode

Returns

0 - exit without errors

5.2 src/coords.c File Reference

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

Functions

- int reading_coords (const int mode, const char ∗filename, const int type_inter, const int ∗label_atom, const float ∗cell, int ∗num_mol, int ∗num_atoms, int ∗true_label_mol, int ∗label_mol, int ∗type_atoms, float ∗coords, char ∗ch_type_atoms)

  function that reads coordinates from special file format

5.2.1 Function Documentation

5.2.1.1 int reading_coords (const int *mode,* const char ∗ *filename,* const int *type_inter,* const int ∗ *label_atom,* const float ∗ *cell,* int ∗ *num_mol,* int ∗ *num_atoms,* int ∗ *true_label_mol,* int ∗ *label_mol,* int ∗ *type_atoms,* float ∗ *coords,* char ∗ *ch_type_atoms*)

function that reads coordinates from special file format

```
* reading_coords (0, filename, type_inter, label_atom, cell, &num_mol, &num_atoms,
*                 true_label_mol, label_mol, type_atoms, coords, ch_type_atoms);
*
```

Parameters

mode	mode of reading; '1' is statgen, '2' is envir or frad, '3' is agl
filename	input file name
type_inter	number of needed atoms (number of needed molecules)
label_atom	massive of needed atom types (massive of needed molecules)
cell	massive of cell size
num_mol	number of molecules
num_atoms	number of atoms
true_label_mol	massive of true numbers of molecule for atoms
label_mol	massive of numbers of molecule for atoms
type_atoms	massive of atom types
coords	massive of coordinates
ch_type_atoms	massive of char atom types

Returns

1 - file $filename does not exist
2 - unknown mode
0 - exit without errors

Work blocks

```
reading file

translation

free memory
```

5.3 src/main.c File Reference

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include "add_main.h"
#include "coords.h"
#include "messages.h"
#include "print_struct.h"
```

Functions

- int main (int argc, char ∗argv[])

5.3.1 Function Documentation

5.3.1.1 int main (int *argc,* char ∗ *argv[]*)

Returns

1 - error in error_checking
2 - input file does not exist
3 - memory error
4 - unknown flag
0 - exit without errors

5.4 src/messages.c File Reference

```
#include <stdio.h>
#include <time.h>
```

Functions

- int message (const int log, const int mode, const char ∗text, FILE ∗output)

  function that prints messages to output

5.4.1 Function Documentation

5.4.1.1 int message (const int *log,* const int *mode,* const char ∗ *text,* FILE ∗ *output*)

function that prints messages to output

```
* message (log, mode, text, output);
*
```

Parameters

log	equal to 1 if print to logfile
mode	number of message
text	additional text
output	output file (may be stdout)

Returns

1 - unknown mode
0 - exit without errors

5.5 src/print_struct.c File Reference

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

Functions

- int print_structure (const char ∗output, const int num_needed_mol, const int ∗needed_mol, const int num_atoms, const int ∗label_mol, const char ∗ch_type_atoms, const float ∗coords)

  function that prints structure to pdb file

5.5.1 Function Documentation

5.5.1.1 int print_structure (const char ∗ *output*, const int *num_needed_mol*, const int ∗ *needed_mol*, const int *num_atoms*, const int ∗ *label_mol*, const char ∗ *ch_type_atoms*, const float ∗ *coords*)

function that prints structure to pdb file

```
* print_structure (output, num_needed_mol, needed_mol, num_atoms, label_mol,
*                  char_type_atoms, coords);
*
```

Parameters

output	output file name
num_needed_-mol	number of needed molecules
needed_mol	massive of number of needed molecules
num_atoms	number of atoms
label_mol	massive of numbers of molecule for atoms
ch_type_atoms	massive of char atom types
coords	massive of coordinates

Returns

0 - exit without errors

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