

fpocket

1.0

Generated by Doxygen 1.5.9

Sun Jul 5 15:08:38 2009

Contents

1	Data Structure Index	1
1.1	Data Structures	1
2	Data Structure Documentation	3
2.1	node_vertice Struct Reference	3
2.1.1	Detailed Description	3
2.2	ptr_node Struct Reference	5
2.2.1	Detailed Description	5
2.3	s_amino_a Struct Reference	6
2.3.1	Detailed Description	6
2.4	s_atm Struct Reference	7
2.4.1	Detailed Description	7
2.5	s_desc Struct Reference	9
2.5.1	Detailed Description	9
2.6	s_fparams Struct Reference	11
2.6.1	Detailed Description	11
2.7	s_vect_elem Struct Reference	12
2.7.1	Detailed Description	12
2.8	s_vsort Struct Reference	13
2.8.1	Detailed Description	13

Chapter 1

Data Structure Index

1.1 Data Structures

Here are the data structures with brief descriptions:

node_vertice	3
ptr_node	5
s_amino_a	6
s_atm	7
s_desc	9
s_fparams	11
s_vect_elem	12
s_vsort	13

Chapter 2

Data Structure Documentation

2.1 node_vertice Struct Reference

```
#include <voronoi_lst.h>
```

Data Fields

- struct `node_vertice` * `next`
- struct `node_vertice` * `prev`
- `s_vvertice` * `vertice`

2.1.1 Detailed Description

COPYRIGHT DISCLAIMER

Vincent Le Guilloux, Peter Schmidtke and Pierre Tuffery, hereby disclaim all copyright interest in the program “fpocket” (which performs protein cavity detection) written by Vincent Le Guilloux and Peter Schmidtke.

Vincent Le Guilloux 28 November 2008 Peter Schmidtke 28 November 2008 Pierre Tuffery 28 November 2008

GNU GPL

This file is part of the fpocket package.

fpocket is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

fpocket is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

You should have received a copy of the GNU General Public License along with fpocket. If not, see <http://www.gnu.org/licenses/>.

Definition at line 54 of file voronoi_lst.h.

The documentation for this struct was generated from the following file:

- `/home/peter/ETUDES/fpocket/fpocket_svn/dev/headers/voronoi_lst.h`

2.2 ptr_node Struct Reference

Data Fields

- struct [ptr_node](#) * next
- void * ptr

2.2.1 Detailed Description

```
## — GENERAL INFORMATION ## ## FILE memhandler.h ## AUTHORS P. Schmidtke and V. Le  
Guilloux ## LAST MODIFIED 28-11-08 ## ## — SPECIFICATIONS ## ## This file implements a  
memory handler. Whenever you call ## my_bloc_malloc function, the allocated pointer will be ## stored  
in a simple chained list. Then, if a malloc fails, ## or if you call the my_exit function, all allocated variable  
## will be freed if not NULL of course. Therefore, a bloc ## allocated by my_... functions MUST be  
freed by the my_free, ## or a double free error should appears. ## ## WARNING ## ## This is an easy  
way to handle memory. However, if many bloc ## are allocated and removed during the programm, it  
might be ## solwed down as for each free, as we have to look for the bloc ## to free in the list, and  
remove it. ## ## REMEMBER: if you use my_malloc, you MUST use my_free. If you ## free a bloc  
allocated by my_(..), and if you call free_all at ## the end, a double free coprruption will occure. ## ##  
— MODIFICATIONS HISTORY ## ## 28-11-08 (v) Comments UTD ## 01-04-08 (v) Added comments  
and creation of history ## 01-01-08 (vp) Created (random date...) ## ## — TODO or SUGGESTIONS  
## COPYRIGHT DISCLAIMER
```

Vincent Le Guilloux, Peter Schmidtke and Pierre Tuffery, hereby disclaim all copyright interest in the program “fpocket” (which performs protein cavity detection) written by Vincent Le Guilloux and Peter Schmidtke.

Vincent Le Guilloux 28 November 2008 Peter Schmidtke 28 November 2008 Pierre Tuffery 28 November 2008

GNU GPL

This file is part of the fpocket package.

fpocket is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

fpocket is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

You should have received a copy of the GNU General Public License along with fpocket. If not, see <http://www.gnu.org/licenses/>.

Definition at line 79 of file memhandler.c.

The documentation for this struct was generated from the following file:

- /home/peter/ETUDES/fpocket/fpocket_svn/dev/src/memhandler.c

2.3 s_amino_a Struct Reference

```
#include <aa.h>
```

Data Fields

- char **name3** [4]
- char **code**
- float **mw**
- float **volume**
- float **hydrophobicity**
- int **charge**
- int **polarity**
- int **func_grp**

2.3.1 Detailed Description

A structure for the modelisation of an amino acid

Definition at line 70 of file aa.h.

The documentation for this struct was generated from the following file:

- /home/peter/ETUDES/fpocket/fpocket_svn/dev/headers/aa.h

2.4 s_atm Struct Reference

```
#include <atom.h>
```

Data Fields

- int **sort_x**
- float **x**
- float **y**
- float **z**
- char **name** [5]
- char **type** [7]
- char **chain** [2]
- char **symbol** [3]
- char **res_name** [8]
- int **id**
- int **seen**
- int **res_id**
- int **atype**
- int **charge**
- float **mass**
- float **radius**
- float **electroneg**
- float **occupancy**
- float **bfactor**
- char **pdb_insert**
- char **pdb_aloc**
- int **atomic_num**

2.4.1 Detailed Description

COPYRIGHT DISCLAIMER

Vincent Le Guilloux, Peter Schmidtke and Pierre Tuffery, hereby disclaim all copyright interest in the program “fpocket” (which performs protein cavity detection) written by Vincent Le Guilloux and Peter Schmidtke.

Vincent Le Guilloux 28 November 2008 Peter Schmidtke 28 November 2008 Pierre Tuffery 28 November 2008

GNU GPL

This file is part of the fpocket package.

fpocket is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

fpocket is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

You should have received a copy of the GNU General Public License along with fpocket. If not, see <http://www.gnu.org/licenses/>.

Definition at line 52 of file atom.h.

The documentation for this struct was generated from the following file:

- /home/peter/ETUDES/fpocket/fpocket_svn/dev/headers/atom.h

2.5 s_desc Struct Reference

```
#include <descriptors.h>
```

Data Fields

- float **hydrophobicity_score**
- float **volume_score**
- float **volume**
- float **prop_polar_atm**
- float **mean_asph_ray**
- float **masph_sacc**
- float **apolar_asphere_prop**
- float **mean_loc_hyd_dens**
- float **as_density**
- float **as_max_dst**
- float **flex**
- float **nas_norm**
- float **polarity_score_norm**
- float **mean_loc_hyd_dens_norm**
- float **prop_asapol_norm**
- float **as_density_norm**
- float **as_max_dst_norm**
- int **aa_compo** [20]
- int **nb_asph**
- int **polarity_score**
- int **charge_score**
- float **as_max_r**

2.5.1 Detailed Description

COPYRIGHT DISCLAIMER

Vincent Le Guilloux, Peter Schmidtke and Pierre Tuffery, hereby disclaim all copyright interest in the program “fpocket” (which performs protein cavity detection) written by Vincent Le Guilloux and Peter Schmidtke.

Vincent Le Guilloux 28 November 2008 Peter Schmidtke 28 November 2008 Pierre Tuffery 28 November 2008

GNU GPL

This file is part of the fpocket package.

fpocket is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

fpocket is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

You should have received a copy of the GNU General Public License along with fpocket. If not, see <http://www.gnu.org/licenses/>.

Definition at line 52 of file descriptors.h.

The documentation for this struct was generated from the following file:

- /home/peter/ETUDES/fpocket/fpocket_svn/dev/headers/descriptors.h

2.6 s_fparams Struct Reference

```
#include <fparams.h>
```

Data Fields

- char **pdb_path** [M_MAX_PDB_NAME_LEN]
- char ** **pdb_lst**
- int **npdb**
- int **min_apol_neigh**
- int **sl_clust_min_nneigh**
- int **nb_mcv_iter**
- int **basic_volume_div**
- int **min_pock_nb_asph**
- float **clust_max_dist**
- float **refine_min_apolar_asphere_prop**
- float **sl_clust_max_dist**
- float **refine_clust_dist**
- float **asph_min_size**
- float **asph_max_size**

2.6.1 Detailed Description

Structure containing all necessary parameters that can be changed by the user. This structure is commun to both programs (validation and pocket finding), even if the pocked finding programm doesn't need some parameters.

Definition at line 143 of file fparams.h.

The documentation for this struct was generated from the following file:

- /home/peter/ETUDES/fpocket/fpocket_svn/dev/headers/fparams.h

2.7 s_vect_elem Struct Reference

```
#include <sort.h>
```

Data Fields

- void * **data**
- int **type**

2.7.1 Detailed Description

A vector (here it will be either atoms or vertices)

Definition at line 63 of file sort.h.

The documentation for this struct was generated from the following file:

- /home/peter/ETUDES/fpocket/fpocket_svn/dev/headers/sort.h

2.8 s_vsort Struct Reference

```
#include <sort.h>
```

Data Fields

- [s_vect_elem](#) * **xsort**
- int **nelem**

2.8.1 Detailed Description

A list of vector (basicly this structure contains atoms and vertices)

Definition at line 73 of file sort.h.

The documentation for this struct was generated from the following file:

- /home/peter/ETUDES/fpocket/fpocket_svn/dev/headers/sort.h

Index

node_vertice, [3](#)

ptr_node, [5](#)

s_amino_a, [6](#)

s_atm, [7](#)

s_desc, [9](#)

s_fparams, [11](#)

s_vect_elem, [12](#)

s_vsort, [13](#)