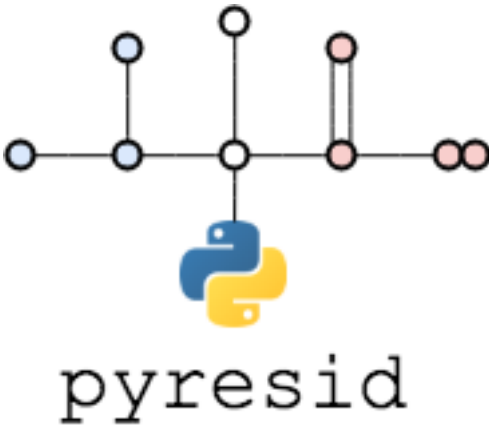

pyresid Documentation

Release 0.2

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CONTENTS:

Python tools for mining Protein Residues from Fulltext articles using PMC number, ePMC and PDB. Identify sentences in structural publications that refer to local features of a protein.

CHAPTER

ONE

HIGH-LEVEL FUNCTIONS

pyresid.**identify_residues**(*fulltext*, *verbose=False*)

Uses Regular Expressions to identify and locate usages of residues within the supplied *fulltext*. Returns a list of MatchClass objects that contain the start and end of the match within the text, and the matched string. For compound matches, a list of positions and residues is included in the match, which needs decomposing before further use.

Parameters

- **fulltext** (*string*) – text to be searched for residues.
- **verbose** (*Bool, optional, default: False*) – Flag to turn on verbose output

Returns **matches** – The matches found within *fulltext*.

Return type List of *MatchClass* objects

See also:

- *locate_residues()*
- *process()*

pyresid.**locate_residues**(*source*, *matches*, *decompose=True*, *nlp=None*, *cifscantype='flex'*, *verbose=True*)

This function takes the raw list of matches from *identify_residues()* and augments them with contextual information and matches them against protein matches also found within the text.

This is a reincarnation of locate_residues2 (despite the name).

Parameters

- **source** (*SourceClass()*) – Class instance containing the source id and fulltext (and possibly the *spaCy* doc)
- **matches** (*List*) – a list of *MatchClass* objects
- **decompose** (*Bool, optional, default: True.*) – Whether to turn the "compound" mentions matched into actual residues.
- **nlp** (spaCy model - https://spacy.io/usage/models, optional, default: None) – The text model to use to turn the *source.fulltext* into *source.doc*
- **verbose** (*Bool, optional, default: False*) – Flag to turn on verbose output

Returns **matches** – The matches found within *fulltext*, augmented with contextual information - sentence, prefix postfix, protein accession id.

Return type List of *MatchClass* objects

pyresid.**process**(*ext_id_list*, *outdir*, *filename='pyresid_output.json'*, *provider='West-Life'*, *cifscantype='flex'*, *save=True*, *overwrite=False*, *return_dict=False*, *decompose=True*, *verbose=False*)

This wraps the main workhorse functions, taking a list of PMC IDs and mining the resulting fulltext. output is a json structure (the encoded output of _locate_residues saved with MyEncoder), to match the EBI specifications.

Parameters

- **ext_id_list** (*List of strings*) – List containing ePMC identifiers used to retrieve the relevant entry. Format is prefix of 'PMC' followed by an integer.
- **outdir** (*String or Path*) – Directory that will contain the output file.
- **filename** (*String*) – The structured output JSON file containing the annotations, one line per *ext_id*.
- **save** (*Bool, optional, default: True*) – Flag to turn off writing the JSON. Good for debugging whenm combined with *return_dict*.
- **overwrite** (*Bool, optional, default: False*) – Flag to determine whether to append (default) or overwrite the json file
- **return_dict** (*Bool, optional, default: False*) – Flag to return the output as a dictionary
- **cifscantype** (*{"flex", "standard"}, default: "flex"*) – Flag passed to *pycifrw* via `_locate_residues2()`; *scantype* can be *standard* or *flex*. *standard* provides pure Python parsing at the cost of a factor of 10 or so in speed. *flex* will tokenise the input CIF file using fast C routines. Note that running PyCIFRW in Jython uses native Java regular expressions to provide a speedup regardless of this argument.
- **context** (*String, optional, default: "sent"*) – Flag passed to `_locate_residues2()` to determine the type of context added to annotations, "sent" uses the spaCy parsed sentences, anything else will use *x* characters either side of the matched tokens.
- **verbose** (*Bool, optional, default: False*) – Flag to turn on verbose output

Returns **(optional) outdict** – Dictionary containing the annotations. Good for debugging.

Return type OrderedDict

See also:

- *locate_residues()*

CHAPTER

TWO

CANDIDATE IDENTIFICATION FUNCTIONS

pyresid.**identify_protein_ID**(*fulltext*, *simple=False*, *infile=None*, *locdir=None*, *verbose=False*)

Uses Regular Expressions to find Protein IDs in the, and then cross-checks against the PDB list of entities.

Parameters

- **fulltext** (*string*) – text snippet to be searched for residues.
- **simple** (*Bool, optional, default: False*) – Flag that, if set, will skip the check against the PDB. Generally a bad idea.
- **infile** (*String or Path, optional, None*) – File to load in order to check candidate PDB entries against. contains the PDB entries - if *None* defaults to "PDBID.list"
- **locdir** (*String or Path, optional, default: None*) – Directory that contains the infile. If None, default is assumed to be *PDB_dir*, if this is not found then will be the user home.
- **verbose** (*Bool, optional, default: False*) – Flag to turn on verbose output

Returns **unique_protiens** – Matches found within *fulltext*

Return type Set

See also:

`_identify_residues()` *load_protein_IDs()*

pyresid.**check_residue_candidate_validity**(*cand*, *pattern='[a-zA-Z]{3}\\d+/\\d+|[a-zA-Z]{3}\\d+'*, *verbose=False*)

Parameters

- **cand** (*String*) – Candidate residue to check for validity
- **pattern** (*String, optional, default : "[a-zA-Z]{3}d+/d+|[a-zA-Z]{3}d+".*) – Regular Expression with which to match the candidate.
- **verbose** (*Bool, optional, default: False*) – Flag to turn on verbose output

Returns **match_bool_list** – List of True/False booleans reflecting the validity of the input candidates.

Return type List of Bool.

CHAPTER

THREE

LOCATION FUNCTIONS

pyresid.**locate_proteins**(*fulltext*, *simple=False*, *infile=None*, *locdir=None*, *verbose=False*)

Uses Regular Expressions to find Protein IDs in the, and then cross-checks against the PDB list of entities. Returns a list of MatchClass objects, rather than a list of strings, as in

Parameters

- **fulltext** (*string*) – text snippet to be searched for residues.
- **simple** (*Bool, optional, default: False*) – Flag that, if set, will skip the check against the PDB. Generally a bad idea.
- **infile** (*String or Path, optional, None*) – File to load in order to check candidate PDB entries against. contains the PDB entries - if *None* defaults to "PDBID.list"
- **locdir** (*String or Path, optional, default: None*) – Directory that contains the infile. If None, default is assumed to be *PDB_dir*, if this is not found then will be the user home.
- **verbose** (*Bool, optional, default: False*) – Flag to turn on verbose output

Returns **matches** – The matches found within *fulltext*.

Return type List of *MatchClass* objects

See also:

- *identify_residues()*
- *load_protein_IDs()*

pyresid.**locate_proteins**(*fulltext*, *simple=False*, *infile=None*, *locdir=None*, *verbose=False*)

Uses Regular Expressions to find Protein IDs in the, and then cross-checks against the PDB list of entities. Returns a list of MatchClass objects, rather than a list of strings, as in

Parameters

- **fulltext** (*string*) – text snippet to be searched for residues.
- **simple** (*Bool, optional, default: False*) – Flag that, if set, will skip the check against the PDB. Generally a bad idea.
- **infile** (*String or Path, optional, None*) – File to load in order to check candidate PDB entries against. contains the PDB entries - if *None* defaults to "PDBID.list"
- **locdir** (*String or Path, optional, default: None*) – Directory that contains the infile. If None, default is assumed to be *PDB_dir*, if this is not found then will be the user home.
- **verbose** (*Bool, optional, default: False*) – Flag to turn on verbose output

Returns **matches** – The matches found within *fulltext*.

Return type List of *MatchClass* objects

See also:

- *identify_residues()*
- *load_protein_IDs()*

CHAPTER

FOUR

API ITERACTION FUNCTIONS

pyresid.**request_fulltextXML**(*ext_id*)

Requests a fulltext XML document from the ePMC REST API. Raises a warning if this is not possible

Parameters **ext_id** (*String*) – ePMC identifier used to retrieve the relevant entry. Format is prefix of 'PMC' followed by an integer.

Returns **r** – The response to the query served up by the requests package.

Return type Requests.Response

pyresid.**parse_request**(*ext_id*)

Wrapper for *request_fulltextXML()* that returns a *BeautifulSoup* XML object

Parameters **ext_id** (*String*) – ePMC identifier used to retrieve the relevant entry. Format is prefix of 'PMC' followed by an integer.

Returns **soup** – BeautifulSoup XML object created from the text response from *pyresid.request_fulltextXML()*

Return type BeautifulSoup

See also:

request_fulltextXML()

CHAPTER

FIVE

OTHER FUNCTIONS

pyresid.**get_sections_text**(*ext_id*, *remove_tables=True*, *fulltext=False*, *verbose=False*)

Requests fulltext XML from the EBI ePMC web REST API, parses the response into a dict.

Parameters

- **ext_id** (*String*) – ePMC identifier used to retrieve the relevant entry. Format is prefix of 'PMC' followed by an integer.
- **remove_tables** (*Bool, optional, default: True*) – Flag to ignore the text found within tables.
- **fulltext** (*Bool, optional, default: False*) – Flag used to return a 'dumb' fulltext (rather than that from *reconstruct_fulltext()*)
- **verbose** (*Bool, optional, default: False*) – Flag to turn on verbose output

Returns **text_dict** – Dictionary containing the parsed XML. Each entry corresponds to a Section in the XML (technically a child of the <*body*>).

Return type OrderedDict

See also:

- *request_fulltextXML()*
- *parse_request()*
- *reconstruct_fulltext()*

pyresid.**reconstruct_fulltext**(*text_dict*, *tokenise=True*, *verbose=False*)

Converts a *text_dict* into a single string or series of tokens in a list of strings.

Parameters

- **text_dict** (*Dict or OrderedDict*) – Dictionary containing the parsed XML. Each entry corresponds to a Section in the XML. Usually an output from *get_sections_text()*
- **tokenise** (*Bool, optional, default: False*) – Flag to enable or disable the reconstructed text being returned as spaCy tokens rather than a string
- **verbose** (*Bool, optional, default: False*) – Flag to turn on verbose output

Returns

- **fulltext** (*string*) – text snippet to be searched for residues.
- *OR*

- **fulltext_tokens** (*List of strings*) – Array of tokens that can be used, for example, to search for *residue_mentions*.

See also:

get_sections_text()

pyresid.**load_protein_IDs**(*infile=None*, *locdir=None*)
Reads in list of valid (approved and pending) PDB entries.

Parameters

- **infile** (*String or Path, optional, default: None*) – File that contains the PDB entries - defaults to "PDBID.list"
- **locdir** (*String or Path, optional, default: None*) – Directory that contains the infile. If None, default is assumed to be *PDB_dir*, if this is not found then will be the user home.

Returns **pdb_arr** – List of valid (approved and pending) PDB entries

Return type List of strings

See also:

- pyresid.combine_compound_IDs()
- pyresid.get_compound_IDfiles()

pyresid.**reconstruct_fulltext**(*text_dict*, *tokenise=True*, *verbose=False*)
Converts a *text_dict* into a single string or series of tokens in a list of strings.

Parameters

- **text_dict** (*Dict or OrderedDict*) – Dictionary containing the parsed XML. Each entry corresponds to a Section in the XML. Usually an output from *get_sections_text()*
- **tokenise** (*Bool, optional, default: False*) – Flag to enable or disable the reconstructed text being returned as spaCy tokens rather than a string
- **verbose** (*Bool, optional, default: False*) – Flag to turn on verbose output

Returns

- **fulltext** (*string*) – text snippet to be searched for residues.
- *OR*
- **fulltext_tokens** (*List of strings*) – Array of tokens that can be used, for example, to search for *residue_mentions*.

See also:

get_sections_text()

pyresid.**get_text**(*ext_id*, *verbose=False*)
A wrapper for *get_sections_text()* that adds additional information to the *text_dict*.

Parameters

- **ext_id** (*String*) – ePMC identifier used to retrieve the relevant entry. Format is prefix of 'PMC' followed by an integer.
- **verbose** (*Bool, optional, default: False*) – Flag to turn on verbose output

Returns **text_dict** – Dictionary containing the parsed XML. Each entry corresponds to a Section in the XML (technically a child of the <*body*>). An augmented version of the *text_dict* returned by *get_sections_text()* - containing additional information including spaCy tokens, length in characters and starting offset.

Return type OrderedDict

See also:

- *get_sections_text()*

pyresid.**setup_plot_defaults**()
Sets up default plot settings for figures.

CHAPTER

SIX

CLASSES

class pyresid.**SourceClass**
Class for handling sources

class pyresid.**MatchClass**(*start*, *end*, *string*)
Class for handling residue matches.

class pyresid.**ProteinMatchClass**(*start*, *end*, *string*)
Class for handling protein structure matches

class pyresid.**MyEncoder**(*, *skipkeys=False*, *ensure_ascii=True*, *check_circular=True*, *allow_nan=True*, *sort_keys=False*, *indent=None*, *separators=None*, *default=None*)

CHAPTER

SEVEN

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CHAPTER

EIGHT

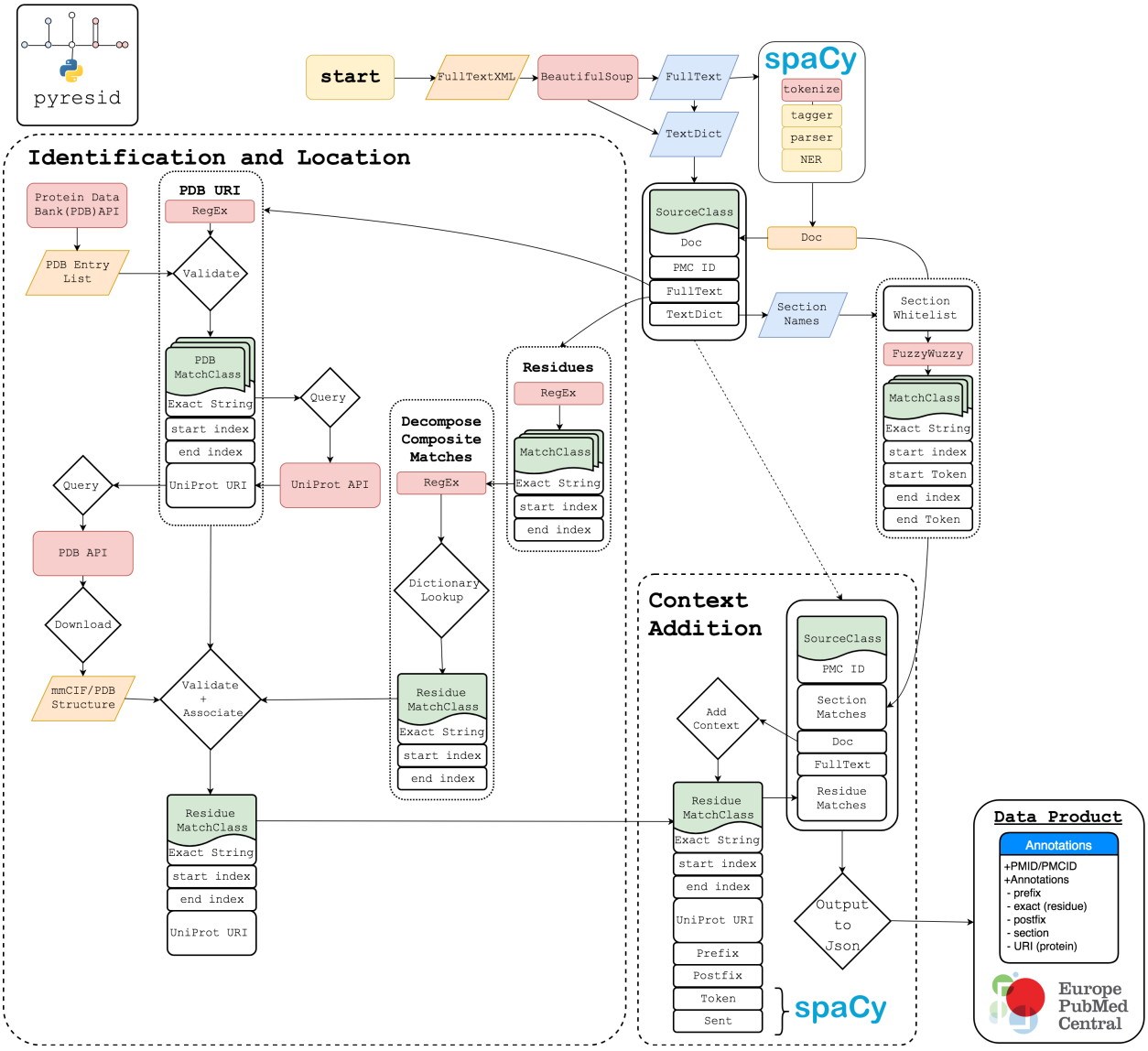
INDICES AND TABLES

- genindex
- modindex
- *License*
- search

CHAPTER

NINE

STRUCTURE



INDEX