Package ‘CellaRepertorium’

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Type Package

Title Data structures, clustering and testing for single cell immune receptor repertoires (scRNAseq RepSeq/AIRR-seq)

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Description Methods to cluster and analyze high-throughput single cell immune cell repertoires, especially from the 10X Genomics VDJ solution. Contains an R interface to CD-HIT (Li and Godzik 2006). Methods to visualize and analyze paired heavy-light chain data. Tests for specific expansion, as well as omnibus oligoclonyality under hypergeometric models.

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R topics documented:

.cluster_permute_test .......................................................... 3
canonicalize_cell .............................................................. 4
canonicalize_cluster ............................................................ 5
ccdb_ex ............................................................... 7
ccdb_join ............................................................... 7
cdhit .............................................................. 8
cdhit_ccdb .............................................................. 9
cland ............................................................... 10
cluster_filterset ............................................................ 11
cluster_germline .............................................................. 12
cluster_permute_test ............................................................ 12
cluster_plot ............................................................... 14
cluster_test_by .............................................................. 15
ContigCellDB ............................................................... 16
contigs_qc ............................................................... 18
crosstab_by_celltype ............................................................. 19
cross_tab_tbl .............................................................. 19
entropy ................................................................. 20
equalize_ccdb .............................................................. 21
fancy_name_contigs ............................................................. 22
filter_cdb ............................................................... 23
fine_clustering .............................................................. 24
fine_cluster_seqs ............................................................. 25
generate_pseudobulk ............................................................ 26
Description

Cell permutation tests (internal)

Usage

.cluster.permute_test(
  labels,
  covariates,
  strata,
  statistic,
  contrasts,
  n_perm,
  alternative,
  ...
)

Arguments

labels factor of length n
covariates data.frame of length n
strata factor
statistic function of label (vector) and covariate (data.frame). If this returns a vector, then by default each level will be compared against each other, pairwise, but see the next section.
canonicalize_cell

contrasts an optional list of numeric vectors. Each will be dotted with the statistic, or optionally a matrix provided in which case each row would be tested one-by-one.

n_perm number of permutations to run

alternative character naming the direction statistic should be fall under the alternative hypothesis

... passed along to statistic

Value

a list containing the observed value of the statistic, the permuted values of the statistic, its expectation (under independence), a p-value, and the Monte Carlo standard error (of the expected value).

---

canonicalize_cell Find a canonical contig to represent a cell

Description

Using filtering in contig_filter_args and sorting in tie_break_keys and order find a single, canonical contig to represent each cell Fields in contig_fields will be copied over to the cell_tbl.

Usage

canonicalize_cell(
  ccdb,
  contig_filter_args = TRUE,
  tie_break_keys = c("umis", "reads"),
  contig_fields = tie_break_keys,
  order = 1,
  overwrite = TRUE
)

Arguments

ccdb ContigCellDB() contig_filter_args

an expression passed to dplyr::filter(). Unlike filter, multiple criteria must be & together, rather than using commas to separate. These act on ccdb$contig_tbl

tie_break_keys (optional) character naming fields in contig_tbl that are used sort the contig table in descending order. Used to break ties if contig_filter_args does not return a unique contig for each cluster

contig_fields Optional fields from contig_tbl that will be copied into the cluster_tbl from the canonical contig.
**canonicalize_cluster**

Find a canonical contig to represent a cluster

**Description**

Find a canonical contig to represent a cluster

**Usage**

```
canonicalize_cluster(
  ccdb,
  contig_filter_args,
  tie_break_keys = character(),
  order = 1,
  representative = ccdb$cluster_pk[1],
)
```
canonicalize_cluster

```r
ccontig_fields = c("cdr3", "cdr3_nt", "chain", "v_gene", "d_gene", "j_gene"),
overwrite = TRUE
)
```

### Arguments

- **ccdb**
  - `ContigCellDB()`
- **contig_filter_args**
  - An expression passed to `dplyr::filter()`. Unlike `filter`, multiple criteria must be & together, rather than using commas to separate. These act on `ccdb$contig_tbl`
- **tie_break_keys**
  - (optional) character naming fields in `contig_tbl` that are used sort the contig table in descending order. Used to break ties if `contig_filter_args` does not return a unique contig for each cluster
- **order**
  - The rank order of the contig based on `tie_break_keys` to return. If `tie_break_keys` included an ordered factor (such as `chain`) this could be used to return the second chain.
- **representative**
  - An optional field from `contig_tbl` that will be made unique. Serve as a surrogate `cluster_pk`.
- **contig_fields**
  - Optional fields from `contig_tbl` that will be copied into the `cluster_tbl` from the canonical contig.
- **overwrite**
  - Logical – should non-key fields in `y` be overwritten using `x`, or should a suffix (".y") be added

### Value

`ContigCellDB()` with some number of clusters/contigs/cells but with "canonical" values copied into `cluster_tbl`

### See Also

- `canonicalize_cell()`
- `left_join_warn()`

### Examples

```r
library(dplyr)
data(ccdb_ex)
ccdb_ex_small = ccdb_ex
ccdb_ex_small$cell_tbl = ccdb_ex_small$cell_tbl[1:200,]
ccdb_ex_small = cdhit_ccdb(ccdb_ex_small, 
sequence_key = 'cdr3_nt', type = 'DNA', cluster_name = 'DNA97',
identity = .965, min_length = 12, G = 1)
ccdb_ex_small = fine_clustering(ccdb_ex_small, sequence_key = 'cdr3_nt', type = 'DNA')

# Canonicalize with the medoid contig is probably what is most common
ccdb_medoid = canonicalize_cluster(ccdb_ex_small)

# But there are other possibilities.
# To pass multiple "AND" filter arguments must use &
```
ccdb_ex

ccdb_umi = canonicalize_cluster(ccdb_ex_small,
    contig_filter_args = chain == 'TRA' & length > 500, tie_break_keys = 'umis',
    contig_fields = c('chain', 'length'))
ccdb_umi$cluster_tbl %>% dplyr::select(chain, length) %>% summary()

---

**Description**

A preconstructed ContigClusterDB from the contigs_qc data

**Usage**

data(ccdb_ex)

**Format**

ccdb_ex = ContigCellDB_10XVDJ(contigs_qc, contig_pk = c('pop', 'sample', 'barcode',
    'contig_id'), cell_pk = c('pop', 'sample', 'barcode'))

**See Also**

contigs_qc

---

**ccdb_join**

Join dataframe or SingleCellExperiment object with ContigCellDB object

**Description**

Join dataframe or SingleCellExperiment object with ContigCellDB object

**Usage**

ccdb_join(template, ccdb, join_fun = dplyr::left_join, by = ccdb$cell_pk)

**Arguments**

- `template` : data.frame or SingleCellExperiment object to be joined with ccdb.
- `ccdb` : A ContigCellDB object.
- `join_fun` : Function used for the join operation.
- `by` : A character vector of variables to join by.
Value

`ContigCellDB()`

Examples

data(ccdb_ex)

to_join = dplyr::bind_rows(ccdb_ex$cell_tbl[1:10,],
                        dplyr::tibble(barcode = c('extra1', 'extra2'), sample = LETTERS[1:2],
                                      pop = LETTERS[1:2]))

cdb_join(to_join, ccdb_ex)

cdhit

R interface to CDHIT/CDHITest

Description

CDHIT is a greedy algorithm to cluster amino acid or DNA sequences based on a minimum identity. By default, in this package it is configured to perform ungapped, global alignments with no clipping at start or end. The identity is the number of identical characters in alignment divided by the full length of the shorter sequence. Set s < 1 to change the minimum coverage of the shorter sequence, which will allow clipping at start or end. Changing G = 0 changes the meaning of the identity to be the number of identical characters in the alignment divided by the length of the alignment. In this case, you must also set the alignment coverage controls aL, AL, aS, AS.

Usage

```r
cdhit(
  seqs,
  identity = NULL,
  kmerSize = NULL,
  min_length = 6,
  s = 1,
  G = 1,
  only_index = FALSE,
  showProgress = interactive(),
  ...
)
```

Arguments

- `seqs`: AAseq or DNAseq
- `identity`: minimum proportion identity
- `kmerSize`: word size. If NULL, it will be chosen automatically based on the identity. You may need to lower it below 5 for AAseq with identity less than .7.
- `min_length`: Minimum length for sequences to be clustered. An error if something smaller is passed.
 fraction of shorter sequence covered by alignment.

G  I for global alignment, 0 for local. If doubt, pick global.

only_index  if TRUE only return the integer cluster indices, otherwise return a tibble.

showProgress  show a status bar

...  other arguments that can be passed to cdhit, see https://github.com/weizhongli/cdhit/wiki/3.-User’s-Guide#CDHIT for details. These will override any default values.

CDHit is by Fu, Niu, Zhu, Wu and Li (2012). The R interface is originally by Thomas Lin Pedersen and was transcribed here because it is not exported from the package FindMyFriends, which is orphaned.

vector of integer of length seqs providing the cluster ID for each sequence, or a tibble. See details.

fasta_path = system.file('extdata', 'demo.fasta', package='CellaRepertorium')
aaseq = Biostrings::readAAStringSet(fasta_path)
# 100% identity, global alignment
cdhit(aaseq, identity = 1, only_index = TRUE)[1:10]
# 100% identity, local alignment with no padding of endpoints
cdhit(aaseq, identity = 1, G = 0, aL = 1, aS = 1, only_index = TRUE)[1:10]
# 100% identity, local alignment with .9 padding of endpoints
cdhit(aaseq, identity = 1, G = 0, aL = .9, aS = .9, only_index = TRUE)[1:10]
# a tibble
tbl = cdhit(aaseq, identity = 1, G = 0, aL = .9, aS = .9, only_index = FALSE)
Arguments

- **ccdb**: An object of class `ContigCellDB`
- **sequence_key**: character naming the column in the `contig_tbl` containing the sequence to be clustered
- **type**: one of 'DNA' or 'AA'
- **cluster_pk**: character specifying key, and name for the clustering.

Arguments passed on to `cdhit`

- **identity**: minimum proportion identity
- **kmerSize**: word size. If NULL, it will be chosen automatically based on the identity. You may need to lower it below 5 for AAseq with identity less than .7.
- **min_length**: Minimum length for sequences to be clustered. An error if something smaller is passed.
- **s**: fraction of shorter sequence covered by alignment.
- **showProgress**: show a status bar
- **G**: 1 for global alignment, 0 for local. If doubt, pick global.

Value

`ContigCellDB`

See Also

`cdhit()`

Examples

```r
data(ccdb_ex)
res = cdhit_ccdb(ccdb_ex, 'cdr3_nt', type = 'DNA',
cluster_name = 'DNA97', identity = .965, min_length = 12, G = 1)
res$cluster_tbl
res$contig_tbl
res$cluster_pk
```

---

**cland**

*Cluster "And" intersection*

Description

For each contig present in both \(X\) and \(Y\), a new cluster is defined that combines cluster identities in both \(X\) and \(Y\). In the resulting `ContigCellDB`, two contigs are in the same cluster if they are in the same cluster in \(X\) and the same cluster in \(Y\). \(X\) and \(Y\) must have matching `contig_pk`. The `contig_tbl` has fields from \(X\) for contigs present in both \(X\) and \(Y\). The `cell_tbl` from \(X\) is carried forward unchanged, while the `cluster_tbl` in the result contains the mapping between the ancestral clustering, and the derived.
**Usage**

`cland(X, Y, new_pk)`

**Arguments**

- **X**: ContigCellDB
- **Y**: ContigCellDB
- **new_pk**: optional character naming the new pk.

**Examples**

```r
data(ccdb_ex)
ccdb_germ = cluster_germline(ccdb_ex, cluster_pk = 'germline_idx')
ccdb_cdr3 = cdhit_ccdb(ccdb_ex, 'cdr3_nt', type = 'DNA',
  cluster_name = 'DNA97', identity = .965, min_length = 12, G = 1)
ccdb_cdr3 = cland(ccdb_cdr3, ccdb_germ)
```

---

**cluster_filterset**  
*A filtration of clusters*

**Description**

Return clusters that match all provided conditions

**Usage**

`cluster_filterset(min_number = 0, min_freq = 0, white_list = NULL)`

**Arguments**

- **min_number**: integer At least this many cells
- **min_freq**: numeric At least this frequency
- **white_list**: data.frame keyed by cluster_pk that must match

**Value**

object representing the filtration (currently a list)

**Examples**

```r
cluster_filterset(min_number = 1, min_freq = 0)
```
**cluster_germline**  
*Cluster contigs by germline properties*

**Description**

Cluster contigs by germline properties

**Usage**

```r
closest_rotation:
  cluster_germline(
    ccdb,
    segment_keys = c("v_gene", "j_gene", "chain"),
    cluster_pk = "cluster_idx"
  )
```

**Arguments**

- `ccdb`  
  ContigCellDB()
- `segment_keys`  
  fields in contig_tbl that identify a cluster
- `cluster_pk`  
  name of cluster to be added to cluster_tbl

**Value**

ContigCellDB()

**Examples**

```r
data(ccdb_ex)
ccdb_ex = cluster_germline(ccdb_ex)
ccdb_ex$cluster_tbl
```

**cluster_permute_test**  
*Tests for independence between labels and covariates using permutation of cells*

**Description**

This tests a statistic for association between labels (for instance, cluster/clonal ID) and covariates (for instance, subject or treatment) by permuting the link between the two. Each observation represents a cell. statistic is any function of labels.
Usage

```r
cluster_permute_test(
  ccdb,
  cell_covariate_keys,
  cell_label_key = ccdb$cluster_pk,
  cell_stratify_keys,
  statistic,
  contrasts = NULL,
  n_perm,
  alternative = c("two-sided", "less", "greater"),
  sanity_check_strata = TRUE,
  ...
)
```

Arguments

- `ccdb` ContigCellDB
- `cell_covariate_keys` character naming fields in `ccdb$cell_tbl`
- `cell_label_key` character naming a single field in `ccdb$cell_tbl`
- `cell_stratify_keys` optional character naming fields in `ccdb$cell_tbl` under which permutations of `cell_label_key` will occur. This means that the test will occur conditional on these covariates. Must be disjoint from `cell_covariate_keys`.
- `statistic` function of label (vector) and covariate (data.frame). If this returns a vector, then by default each level will be compared against each other, pairwise, but see the next section.
- `contrasts` an optional list of numeric vectors. Each will be dotted with the statistic, or optionally a matrix provided in which case each row would be tested one-by-one.
- `n_perm` number of permutations to run
- `alternative` character naming the direction statistic should be fall under the alternative hypothesis
- `sanity_check_strata` logical, should `cell_stratify_keys` be checked for sanity?
- `...` passed to `statistic`

Value

a list containing the observed value of the statistic, the permuted values of the statistic, its expectation (under independence), a p-value, and the Monte Carlo standard error (of the expected value).

See Also

`purity()`
Examples

```r
library(dplyr)
# covariate should name one or more columns in `cell_tbl`

cluster_idx = c(1, 1, 1, 2, 2, 3, 3)
subject = c('A', 'A', 'B', 'B', 'C', 'C')
contig_tbl = tibble(contig_pk = seq_along(cluster_idx), cluster_idx, subject)
ccdb_test = ContigCellDB(contig_tbl = contig_tbl, contig_pk = 'contig_pk',
cell_pk = c('contig_pk', 'subject', 'cluster_idx'), cluster_pk = 'cluster_idx')
ccdb_test$cell_tbl

clust_test = cluster_permute_test(ccdb_test, 'subject', 'cluster_idx',
statistic = purity, n_perm = 50)
library(ggplot2)
plot_permute_test(perm_test = clust_test)
tidy.PermuteTest(clust_test)
```

---

cluster_plot

Make a plot showing properties of the clustering

Description

The number of elements per cluster and the average distance between the medoid and other elements are plotted.

Usage

```r
cluster_plot(cdb, return_plotlist = FALSE)
```

Arguments

- `cdb` A fine_clustering ContigCellDB object
- `return_plotlist` should a list of ggplot2 plots be returned. If FALSE, a cowplot composite is returned.

Value

a cowplot composite or a list of plots.

Examples

```r
library(dplyr)
data(ccdb_ex)
ccdb_ex_small = ccdb_ex
ccdb_ex_small$cell_tbl = ccdb_ex_small$cell_tbl[1:200,]
ccdb_ex_small = cdhit_ccdb(ccdb_ex_small, sequence_key = 'cdr3_nt', type = 'DNA', cluster_name = 'DNA97', identity = .965, min_length = 12, G = 1)
```
**cluster_test_by**

Typically one will want to stratify by chain by calling `cluster_test_by`, as this will calculate the number of cell “trials” separately depending on the chain recovered.

### Usage

```r
code

cluster_test_by(ccdb, fields = "chain", tbl = "cluster_tbl", ...)  
```

### Arguments

- **ccdb**
  - ContigCellDB()
- **fields**
  - character naming fields in tbl
- **tbl**
  - one of contig_tbl, cell_tbl or cluster_tbl
- **formula**
  - the right-hand side of a glmer or glm-style formula.
- **filterset**
  - a call to `cluster_filterset()` that will be used to subset clusters.
contig_filter_args
an expression passed to \texttt{dplyr::filter()}. Unlike filter, multiple criteria must be \& together, rather than using commas to separate. These act on ccdb$contig_tbl

tie_break_keys (optional) character naming fields in contig_tbl that are used sort the contig table in descending order. Used to break ties if contig_filter_args does not return a unique contig for each cluster

add_cluster_tbl
logical should the output be joined to the cluster_tbl?

keep_fit logical as to whether the fit objects should be returned as a list column

fitter a function taking arguments \texttt{formula, data, is_mixed} and \texttt{keep_fit} that is run on each cluster. Should return a tibble or \texttt{data.frame}

silent logical. Should warnings from fitting functions should be suppressed?

Value
table with one row per cluster/term.

Functions

- \texttt{cluster_test_by}: split ccdb and conduct tests within strata

Examples

```r
library(dplyr)
data(ccdb_ex)
ccdb_ex = cluster_germline(ccdb_ex)
trav1 = filter(ccdb_ex$cluster_tbl, v_gene == 'TRAV1')
cluster_logistic_test(~pop + (1|sample), ccdb_ex,
filterset = cluster_filterset(white_list= trav1))
# Fixed effect analysis of each cluster, by chain
prev4 = ccdb_ex$contig_tbl %>% group_by(cluster_idx) %>%
summarize(n()) %>% filter(`n()`>= 4)
cluster_test_by(ccdb = ccdb_ex, fields = 'chain',
tbl = 'cluster_tbl', formula = ~ pop, filterset = cluster_filterset(white_list= prev4))
```

---

ContigCellDB

Construct a ContigCellDB

Description

Construct a ContigCellDB
Usage

ContigCellDB(
  contig_tbl,
  contig_pk,
  cell_tbl,
  cell_pk,
  cluster_tbl,
  cluster_pk = character(),
  equalize = TRUE
)

ContigCellDB_10XVDJ(
  contig_tbl,
  contig_pk = c("barcode", "contig_id"),
  cell_pk = "barcode",
  ...
)

Arguments

contig_tbl a data frame of contigs, and additional fields describing their properties
contig_pk character vector naming fields in contig_tbl that uniquely identify a row/contig
cell_tbl a data frame of cell barcodes, and (optional) additional fields describing their properties
cell_pk character vector naming fields in cell_tbl that uniquely identify a cell barcode
cluster_tbl A data frame that provide cluster assignments for each contig
cluster_pk If cluster_tbl was provided, a character vector naming fields in cluster_tbl that uniquely identify a cluster
equalize logical. Should the contig, cells and clusters be equalized by taking the intersection of their common keys?
...
passed to ContigCellDB()

Value

ContigCellDB

Functions

- ContigCellDB_10XVDJ: provide defaults that correspond to identifiers in 10X VDJ data

Accessors/mutators

See $.ContigCellDB-method for more on how to access and mutate slots. See mutate_cdb() and filter_cdb() for endomorphic filtering/mutation methods. See split_cdb() to split into a list, and rbind.ContigCellDB() for the inverse operation.
See Also

\$ContigCellDB\-method

Examples

data(contigs_qc)
contigs_qc
cdb = ContigCellDB(contigs_qc, contig_pk = c('barcode', 'pop', 'sample', 'contig_id'),
cell_pk = c('barcode', 'pop', 'sample'))
cdb

# everything that was in contigs_qc
cdb$contig_tbl

# Only the cell_pk are included by default (until clustering/canonicalization)
cdb$cell_tbl

# Empty, since no cluster_pk was specified
cdb$cluster_tbl

# Keys
cdb$contig_pk
cdb$cell_pk
cdb$cluster_pk

contigs_qc

Filtered and annotated contigs of TCR from mice

Description

Data for c57bl6 and balbc mice TCR were downloaded from 10x Genomics website as shown in
system.file('script/10XMouseTCR_v3_chem.R', package = 'CellaRepertorium'). Additional processing of these data is done in the vignette mouse_tcell_qc and are serialized to serve as examples for other vignettes and documentation.

Usage

data(contigs_qc)

Format

A data frame of 3399 contigs and 22 fields, all except 4 are originally defined in https://support.10xgenomics.com/single-cell-vdj/software/pipelines/latest/output/annotation#contig
The following fields were defined ex post facto.

1. anno_file: Path to original csv file
2. pop: Mouse strain.
3. sample: An artificial "replicate" from the original data defined by subsampling with replacement
4. celltype: The putative cell type of the contig.

---

crosstab_by_celltype  \textit{Count contig UMIs by celltype}

**Description**

Count contig UMIs by celltype

**Usage**

\texttt{crosstab\_by\_celltype(ccdb)}

**Arguments**

- \texttt{ccdb} \hspace{1cm} A ContigCellDB object

**Value**

a table, keyed by \texttt{cell\_pk} counting UMIs per celltype

**See Also**

\texttt{guess\_celltype()}

**Examples**

\begin{verbatim}
data(ccdb_ex)
nrow(ccdb_ex$cell_tbl)
total\_umi = crosstab\_by\_celltype(ccdb_ex)
nrow(total\_umi)
\end{verbatim}

---

cross_tab_tbl \textit{Generate a 2d cross tab using arbitrary numbers of columns as factors}

**Description**

As many rows as unique combs of \texttt{x\_fields} As many columns as unique combs of \texttt{y\_fields} No NA.

**Usage**

\texttt{cross\_tab\_tbl(tbl, x\_fields, y\_fields)}
Arguments

tbl `data.frame`
x_fields `character` fields in tbl
y_fields `character` fields in tbl

Value
tibble

Examples

cross_tab_tbl(mtcars, c('cyl', 'gear'), 'carb')

---

entropy  Calculate the entropy of a vector

Description

Calculate the entropy of a vector

Usage

entropy(v, pseudo_count = length(v)/1000, na.action = na.fail)

np(v, p = 0.05, pseudo_count = p/5, na.action = na.fail)

modal_category(v, na.action = na.fail)

Arguments

v `categorical vector`
pseudo_count number of pseudo counts to add on, to stabilize empty categories
na.action how to handle NA values
p proportion threshold

Value

the sample entropy

Functions

- np: The number of categories exceeding p proportion of the total
- modal_category: The modal category of v. Ties are broken by lexicographic order of the factor levels.
equalize_ccdb

**Examples**

```r
v2 = gl(2, 4)
v4 = gl(4, 4)
stopifnot(entropy(v2) < entropy(v4))
v_empty = v2[1:4] #empty level 2
stopifnot(is.finite(entropy(v_empty))) # pseudo_count

np(v4, p = .2, pseudo_count = 0)
np(v4, p = .25, pseudo_count = 0)
np(v4, p = .25, pseudo_count = .0001)

modal_category(v4)
modal_category(v4[-1])
```

**Description**

The cells in `cell_tbl`, and clusters in `cluster_tbl` can potentially be a superset of the `contig_tbl`.

**Usage**

```r
equalize_ccdb(x, cell = TRUE, contig = TRUE, cluster = TRUE, sort = FALSE)
```

**Arguments**

- `x` `ContigCellDB()`
- `cell` logical equalize cells
- `contig` logical equalize contigs
- `cluster` logical equalize clusters
- `sort` logical should equalized fields also be `order()`ed by their primary keys?

**Details**

- `equalize_ccdb(x, cell = TRUE)` trims cells that aren't in `contig_tbl` or `cluster_tbl`.
- `equalize_ccdb(x, cluster = TRUE)` trims clusters that aren't in `contig_tbl`.
- `equalize_ccdb(x, contig = TRUE)` trims contigs that aren't `cell_tbl` or `cluster_tbl`.

**Value**

`ContigCellDB()`

**Default equalization**

Modification to `contig_tbl` (with `$`) always equalizes contigs and clusters. Modification to `cell_tbl` equalizes only contigs. Modification to `cluster_tbl` equalizes contigs and clusters.
Examples

```r
library(dplyr)
tbl = tibble(clust_idx = gl(3, 2), cell_idx = rep(1:3, times = 2), contig_idx = 1:6)
ccdb = ContigCellDB(tbl, contig_pk = c('cell_idx', 'contig_idx'),
cell_pk = 'cell_idx', cluster_pk = 'clust_idx')
# 3 cells
ccdb
ccdb$cell_tbl = bind_rows(ccdb$cell_tbl, tibble(cell_idx = 0))
# 4 cells now
ccdb
# 3 cells again
equalize_ccdb(ccdb)
# remove all contigs from cell 1, and one contig from cell 2
ccdb$contig_tbl = ccdb$contig_tbl[-c(1, 2, 4),]
# no changes to cell_tbl yet
ccdb
# trim cell_tbl to 2 cells, keep all clusters
equalize_ccdb(ccdb, cluster = FALSE)
# trim both cells and clusters
equalize_ccdb(ccdb, cluster = TRUE)
```

---

**fancy_name_contigs**

*Generate a legible name for a series of contigs*

**Description**

Generate a legible name for a series of contigs

**Usage**

```r
fancy_name_contigs(contig_tbl, prefix)
```

**Arguments**

- `contig_tbl` An `all_contig_annotations.csv` file, output from VDJ Cell ranger. Importantly, this should contain columns `chain, v_gene, d_gene, j_gene`
- `prefix` an optional prefix added to each contig, eg, possibly a sample id.

**Value**

character

**Examples**

```r
library(dplyr)
contig_anno_path = system.file('extdata', 'all_contig_annotations_balbc_1.csv.xz',
package = 'CellaRepertorium')
contig_anno = readr::read_csv(contig_anno_path)
contig_anno = contig_anno %>% mutate(fancy_name =
```
filter_cdb

fancy_name_contigs(., prefix = 'b6_1')
stopifnot(!any(duplicated(contig_anno$fancy_name)))

filter_cdb

Create new or update existing columns of ContigCellDB tables

Description
Create new or update existing columns of ContigCellDB tables

Usage
filter_cdb(ccdb, ..., tbl = "contig_tbl")
mutate_cdb(ccdb, ..., tbl = "contig_tbl")

Arguments
ccdb ContigCellDB()
... name and value pair of column that will be updated
tbl character. One of contig_tbl, cell_tbl or cluster_tbl, naming the table to be updated.

Value
ContigCellDB object with updated table

Functions
• filter_cdb: Filter rows of a table in a ContigCellDB object

See Also
dplyr::mutate()
dplyr::filter()

Examples
data(ccdb_ex)
subset_contig = filter_cdb(ccdb_ex, full_length, productive == 'True',
high_confidence, chain != 'Multi', nchar(cdr3) > 5)
subset_cell = filter_cdb(ccdb_ex, sample == 4, tbl = 'cell_tbl')
data(ccdb_ex)
new_contig = mutate_cdb(ccdb_ex, new_col = 1)
new_cell = mutate_cdb(ccdb_ex, new_col = 1, tbl = 'contig_tbl')
Perform additional clustering of sequences within groups

**Description**

Perform additional clustering of sequences within groups

**Usage**

```r
fine_clustering(
  ccdb,
  sequence_key,
  type,
  max_affinity = NULL,
  keep_clustering_details = FALSE,
  ...
)
```

**Arguments**

- **ccdb**: A `ContigCellDB()` object
- **sequence_key**: character naming column in `contig_tbl` with sequence
- **type**: 'AA' or 'DNA'
- **max_affinity**: numeric naming the maximal affinity for the sparse affinity matrix that is constructed. Not currently used.
- **keep_clustering_details**: logical – should output of `fine_cluster_seqs` be kept as a list column
- **...**: Arguments passed on to `fine_cluster_seqs`
- **big_memory_brute**: attempt to cluster more than 4000 sequences? Clustering is quadratic, so this will take a long time and might exhaust memory
- **method**: one of 'substitutionMatrix' or 'levenshtein'
- **substitution_matrix**: a character vector naming a substitution matrix available in Biostrings, or a substitution matrix itself

**Value**

`ContigCellDB()` object with updated `contig_tbl` and `cluster_tbl`

**Examples**

```r
library(dplyr)
data(ccdb_ex)
ccdb_ex_small = ccdb_ex
ccdb_ex_small$cell_tbl = ccdb_ex_small$cell_tbl[1:200,]
ccdb_ex_small = cdhit_ccdb(ccdb_ex_small,
  sequence_key = 'cdr3_nt',
  type = 'DNA',
  cluster_name = 'DNA97',
...
fine_cluster_seqs

Calculate distances and perform hierarchical clustering on a set of sequences

Description
The distances between AA sequences is defined to be 1-score/max(score) times the median length of the input sequences. The distances between nucleotide sequences is defined to be edit_distance/max(edit_distance) times the median length of input sequences.

Usage
fine_cluster_seqs(
  seqs,
  type = "AA",
  big_memory_brute = FALSE,
  method = "levenshtein",
  substitution_matrix = "BLOSUM100",
  cluster_fun = "none",
  cluster_method = "complete"
)

Arguments
seqs character vector, DNASTRINGSET or-AASTRINGSET
type character either AA or DNA specifying type of seqs
big_memory_brute attempt to cluster more than 4000 sequences? Clustering is quadratic, so this will take a long time and might exhaust memory
method one of 'substitutionMatrix' or 'levenshtein'
substitution_matrix a character vector naming a substitution matrix available in Biostrings, or a substitution matrix itself
cluster_fun character, one of "hclust" or "none", determining if distance matrices should also be clustered with hclust
cluster_method character passed to hclust
generate_pseudobulk

Generate "pseudobulk" data from a ContigCellDB

Description

Tabulate contigs with a unique combination of class_keys per total_keys. For instance, total_keys might be a sample identifier, and class_keys might be the V- and J- gene identities. The idea is that this might mimic the data generated in a bulk experiment.

Usage

generate_pseudobulk(ccdb, class_keys, total_keys, type = c("cell", "umi"))

Arguments

table  
ccdb  
ContigCellDB()
class_keys  character naming fields in contig_tbl that define unique classes of the repertoire
total_keys  character naming fields to be conditioned upon when calculating the total.
type  one of "cell" or "umi"

Details

This function is currently rather 10x-specific, in that it is assumed that columns barcode and umis exist.

Value

tibble

Examples

data(ccdb_ex)
ccdb_ex = cluster_germline(ccdb_ex)
pseudo = generate_pseudobulk(ccdb_ex, c('v_gene', 'j_gene', 'chain'), c('pop', 'sample'))
guess_celltype

Guess the cell type of a contig from the chain ID

Description

This function is likely dependent on annotations from 10X and may change or break as their pipeline changes.

Usage

```r
guess_celltype(chain)
```

Arguments

- `chain` character which will be parsed to try to infer celltype

Value

contig table with celltype column

See Also

crosstab_by_celltype()

Examples

```r
data(ccdb_ex)
table(guess_celltype(ccdb_ex$contig_tbl$chain))
```

hushWarning

Selectively muffle warnings based on output

Description

Selectively muffle warnings based on output

Usage

```
hushWarning(expr, regexp)
```

Arguments

- `expr` an expression
- `regexp` a regexp to be matched (with str_detect)
ig_chain_recode

**Value**

the result of expr

**Examples**

CellaRepertorium:::hushWarning(warning('Beware the rabbit'), 'rabbit')
CellaRepertorium:::hushWarning(warning('Beware the rabbit'), 'hedgehog')

---

**ig_chain_recode**  
*Categorize the pairing present in a cell*

**Description**

For each cell (defined by ccdb$cell_pk) count the number of each level of chain_key occurs, and cross tabulate. Also for each cell, paste together all values chain_key. Return a tibble, keyed by cells that includes the counts of the chains, the raw_chain_type and any additional output from running chain_recode_fun.

**Usage**

ig_chain_recode(tbl)
tcr_chain_recode(tbl)
enumerate_pairing(ccdb, chain_key = "chain", chain_recode_fun = NULL)

**Arguments**

- tbl  
  output from enumerate_pairing containing TRA/TRB or IGH/IHK/IHL columns
- ccdb  
  ContigCellDB
- chain_key  
  character naming the field in the contig_tbl identifying chain
- chain_recode_fun  
  a function that operates on the output of this function that further reduces the chain combinations to some other summary. Set to 'guess' to apply functions that may work for 10X data or NULL to skip. See CellaRepertorium::tcr_chain_recode for an example.

**Value**

a tibble keyed by cells.

**Functions**

- ig_chain_recode: Recode a table with IG chains
- tcr_chain_recode: Recode a table with TCR chains
map_axis_labels

Examples

data(ccdb_ex)
enumerate_pairing(ccdb_ex)
enumerate_pairing(ccdb_ex, chain_recode_fun = 'guess')

map_axis_labels  

Description

Color axis labels

Usage

map_axis_labels(
  plt,  
  label_data_x = NULL,  
  label_data_y = NULL,  
  aes_label,  
  scale = ggplot2::scale_color_hue(aesthetics = "axis_color")
)

Arguments

plt  

label_data_x  

label_data_y  

aes_label  

scale  

Value

plt with axis text modified

Examples

require(ggplot2)
require(dplyr)
plt = ggplot(mpg, aes(x = manufacturer, y = drv)) + geom_jitter()
label_data = mpg %>% select(manufacturer) %>% unique() %>%
  mutate(euro = manufacturer %in% c('audi', 'volkswagen'))
map_axis_labels(plt, label_data_x = label_data, aes_label = euro)
pairing_tables  Generate a list of tables representing clusters paired in cells

Description

A contingency table of every combination of cluster_idx up to table_order is generated. Combinations that are found in at least min_expansion number of cells are reported. All cells that have these combinations are returned, as well as cells that only have orphan_level of matching cluster_idx.

Usage

pairing_tables(
  ccdb,
  ranking_key = "grp_rank",
  table_order = 2,
  min_expansion = 2,
  orphan_level = 1,
  cluster_keys = character(),
  cluster_whitelist = NULL,
  cluster_blacklist = NULL
)

Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ccdb</td>
<td>ContigCellDB</td>
</tr>
<tr>
<td>ranking_key</td>
<td>field in ccdb$contig_tbl giving the ranking of each contig per cell. Probably generated by a call to rank_prevalence_ccdb() or rank_chain_ccdb().</td>
</tr>
<tr>
<td>table_order</td>
<td>Integer larger than 1. What order of cluster_idx will be paired, eg, order = 2 means that the first and second highest ranked contigs will be sought and paired in each cell</td>
</tr>
<tr>
<td>min_expansion</td>
<td>the minimal number of times a pairing needs to occur for it to be reported</td>
</tr>
<tr>
<td>orphan_level</td>
<td>Integer in interval [1, table_order]. Given that at least min_expansion cells are found that have table_order chains identical, how many cluster_idx pairs will we match on to select other cells. Example: orphan_level=1 means that cells that share just a single chain with an expanded pair will be reported.</td>
</tr>
<tr>
<td>cluster_keys</td>
<td>optional character naming additional columns in ccdb$cluster_tbl to be reported in the pairing</td>
</tr>
<tr>
<td>cluster_whitelist</td>
<td>a table of pairings or clusters that should always be reported. Here the clusters must be named &quot;cluster_idx.1&quot;, &quot;cluster_idx.2&quot; (if order-2 pairs are being selected) rather than with ‘ccdb$cluster_pk”</td>
</tr>
<tr>
<td>cluster_blacklist</td>
<td>a table of pairings or clusters that will never be reported. Must be named as per cluster_whitelist.</td>
</tr>
</tbody>
</table>
Details

For example, if `table_order=2` and `min_expansion=2` then heavy/light or alpha/beta pairs found two or more times will be returned (as well as alpha-alpha pairs, etc, if those are present). If `orphan_level=1` then all cells that share just a single chain with an expanded clone will be returned.

The `cluster_idx.1_fct` and `cluster_idx.2_fct` fields in `cell_tbl`, `idx1_tbl`, `idx2_tbl` are cast to factors and ordered such that pairings will tend to occur along the diagonal when they are cross-tabulated. This facilitates plotting.

Value

list of tables. The `cell_tbl` is keyed by the `cell_identifiers`, with fields "cluster_idx.1", "cluster_idx.2", etc, IDing the contigs present in each cell. "cluster_idx.1_fct" and "cluster_idx.2_fct" cast these fields to factors and are reordered to maximize the number of pairs along the diagonal. The `idx1_tbl` and `idx2_tbl` report information (passed in about the cluster_idx by `feature_tbl`). The `cluster_pair_tbl` reports all pairings found of contigs, and the number of times observed.

See Also

`rank_prevalence_ccdb()`

Examples

```r
library(dplyr)
tbl = tibble(clust_idx = gl(3, 2), cell_idx = rep(1:3, times = 2), contig_idx = 1:6)
ccdb = ContigCellDB(tbl, contig_pk = c('cell_idx', 'contig_idx'),
      cell_pk = 'cell_idx', cluster_pk = 'clust_idx')
# add `grp_rank` to ccdb$contig_tbl indicating how frequent a cluster is
ccdb = rank_prevalence_ccdb(ccdb, tie_break_keys = character())
# using `grp_rank` to determine pairing
# no pairs found twice
pt1 = pairing_tables(ccdb)
# all pairs found, found once.
pt2 = pairing_tables(ccdb, min_expansion = 1)
pt2$cell_tbl

tbl2 = bind_rows(tbl, tbl %>% mutate(cell_idx = rep(4:6, times = 2)))
ccdb2 = ContigCellDB(tbl2, contig_pk = c('cell_idx', 'contig_idx'), cell_pk = 'cell_idx',
      cluster_pk = 'clust_idx')
#%>% rank_prevalence_ccdb(tie_break_keys = character())
# all pairs found twice
pt3 = pairing_tables(ccdb2, min_expansion = 1)
pt3$cell_tbl
ccdb2$contig_tbl = ccdb2$contig_tbl %>%
    mutate(umis = 1, reads = 1, chain = rep(c('TRA', 'TRB'), times = 6))
ccdb2 = rank_chain_ccdb(ccdb2, tie_break_keys = character())
pt4 = pairing_tables(ccdb2, min_expansion = 1, table_order = 2)
```
plot_cluster_factors  Visualization of pairs of cluster factor

Description
With factors, a pair of variables present in the contig_tbl and the cluster_tbl, generate and plot cross-tabs of the number of contigs, or its pearson residual.

Usage
plot_cluster_factors(
  ccdb,
  factors,
  type = c("heatmap", "network"),
  statistic = c("pearson", "contigs"),
  ncluster = 0,
  chaintype
)

Arguments
ccdb A ContigCellDB object.
factors character length 2 of fields present
type Type of visualization, a heatmap or a node-edge network plot
statistic Cluster characteristics visualized by pearson residuals or raw contig counts
ncluster integer. Omit factors that occur less than nclusters. For clarity of visualization.
chaintype Character in ccdb$contig_tbl$chain. If passed will subset contigs belonging to specified chain (IGH,IGK,IGL,TRA,TRB)

Value
A ggraph object if type == 'network', and a ggplot object if type == 'heatmap'

See Also
canonicalize_cluster to "roll-up" additional contig variables into the 'cluster_tbl'

Examples
library(ggraph)
data(ccdb_ex)
ccdb_germline_ex = cluster_germline(ccdb_ex, segment_keys = c('v_gene', 'j_gene', 'chain'),
cluster_pk = 'segment_idx')
ccdb_germline_ex = fine_clustering(ccdb_germline_ex, sequence_key = 'cdr3_nt', type = 'DNA')
plot_cluster_factors(ccdb_germline_ex,factors = c('v_gene','j_gene'),
statistic = 'pearson', type = 'network',ncluster = 10, chaintype = 'TRB')
plot_cluster_factors(ccdb_germline_ex, factors = c('v_gene', 'j_gene'), statistic = 'contigs', type = 'heatmap')
plot_cluster_factors(ccdb_germline_ex, factors = c('v_gene', 'j_gene'), statistic = 'contigs', type = 'network', ncluster = 10)

plot_permute_test

Plot a histogram of permuted vs observed test statistic

Description
Plot a histogram of permuted vs observed test statistic

Usage
plot_permute_test(perm_test)
## S3 method for class 'PermuteTestList'
tidy(x, ...)
## S3 method for class 'PermuteTest'
tidy(x, ...)
## S3 method for class 'PermuteTest'
print(x, ...)
## S3 method for class 'PermuteTestList'
print(x, max = 3, ...)

Arguments
perm_test PermuteTest or PermuteTestList output from cluster_permute_test()
x PermuteTestList
... ignored
max maximum number of components to print

Methods (by generic)
• tidy: return permutations run using a sequence of contrasts as a tibble
• tidy: return permutations as a tibble
• print: pretty-print
• print: pretty-print

See Also
cluster_permute_test
purity

*Calculate number of cluster-subject singletons for the purposes of permutation testing*

**Description**

Calculate number of cluster-subject singletons for the purposes of permutation testing

**Usage**

purity(cluster_idx, subject)

**Arguments**

- cluster_idx: factor-like cluster variable
- subject: factor-like subject

**Value**

average number of singletons

**See Also**

cluster_permute_test()

**Examples**

message("see example(cluster_permute_test)")

---

rank_prevalence_ccdb

*Rank contigs, per cell, by experiment-wide prevalence of cluster_pk, which is added as the prevalence field*

**Description**

Rank contigs, per cell, by experiment-wide prevalence of cluster_pk, which is added as the prevalence field
Usage

```r
rank_prevalence_ccdb(
  ccdb,
  contig_filter_args = TRUE,
  tie_break_keys = c("umis", "reads")
)
```

```r
rank_chain_ccdb(
  ccdb,
  contig_filter_args = TRUE,
  tie_break_keys = c("umis", "reads"),
  chain_key = "chain",
  contig_fields = tie_break_keys,
  chain_levels = c("IGL", "IGK", "TRA", "TRB", "IGH")
)
```

Arguments

- `ccdb` ContigCellDB()
- `contig_filter_args` an expression passed to `dplyr::filter()`. Unlike `filter`, multiple criteria must be & together, rather than using commas to separate. These act on `ccdb$contig_tbl`
- `tie_break_keys` (optional) character naming fields in `contig_tbl` that are used sort the contig table in descending order. Used to break ties if `contig_filter_args` does not return a unique contig for each cluster
- `chain_key` character naming the field in `contig_tbl` to be sorted on.
- `contig_fields` Optional fields from `contig_tbl` that will be copied into the `cluster_tbl` from the canonical contig.
- `chain_levels` an optional character vector providing the sort order of the chain column in `tbl`. If set to length zero, then the the ordering will be alphabetical

Value

ContigCellDB with modified `contig_tbl`

Functions

- `rank_chain_ccdb`: return a canonical contig by chain type, with TRB/IGH returned first. By default, ties are broken by umis and reads.

Examples

```r
data(ccdb_ex)
ccdb_ex = cluster_germline(ccdb_ex)
rank_prev = rank_prevalence_ccdb(ccdb_ex)
rank_prev$contig_tbl
rank_chain = rank_chain_ccdb(ccdb_ex)
rank_chain$contig_tbl
```
**Description**

The union of the rows in each of the objects is taken, thus removing any rows that has an exact duplicate. This includes all fields, not just the primary key for that table. The union of the various primary keys is taken.

**Usage**

```r
## S4 method for signature 'ContigCellDB'
rbind(..., deparse.level = 1)
```

**Arguments**

- `...` `ContigCellDB()`
- `deparse.level` ignored

**Value**

`ContigCellDB()`

**Examples**

```r
data(ccdb_ex)
splat = split_cdb(ccdb_ex, 'chain', 'contig_tbl')
unite = equalize_ccdb(rbind(splat$TRA, splat$TRB), sort = TRUE)
stopifnot(all.equal(unite, ccdb_ex))
```

---

**reexports**

*Turn an object into a tidy tibble*

**Description**

*Turn an object into a tidy tibble*

**Usage**

```r
tidy(x, ...)
```

**Arguments**

- `x` An object to be converted into a tidy `tibble::tibble()`.
- `...` Additional arguments to tidying method.
right_join_warn

Value

A `tibble::tibble()` with information about model components.

Methods

No methods found in currently loaded packages.

right_join_warn  
*Perform a dplyr::left_join() but check for non-key overlapping fields*

Description

Perform a dplyr join, but either warn if the two tables share non-key fields If `overwrite = TRUE`, then shared columns will pull from x otherwise a suffix will be added to y. To perform this check, `by` must be specified, and it is an error if it is not.

Usage

right_join_warn(...)

left_join_warn(x, y, by, overwrite = FALSE, join = left_join, ...)

Arguments

...  
passed to joining function

x  
A pair of data frames, data frame extensions (e.g. a tibble), or lazy data frames (e.g. from dbplyr or dtplyr). See Methods, below, for more details.

y  
A pair of data frames, data frame extensions (e.g. a tibble), or lazy data frames (e.g. from dbplyr or dtplyr). See Methods, below, for more details.

by  
character specifying columns in x and y to key on.

overwrite  
logical – should non-key fields in y be overwritten using x, or should a suffix (".y") be added

join  
function giving the type of join to perform, eg, left, right, inner, outer.

Value

data.frame or tibble

Functions

- `right_join_warn`: perform a dplyr::right_join()

Examples

left_join_warn(mtcars, mtcars, by = 'mpg')
left_join_warn(mtcars, mtcars, by = 'mpg', overwrite = TRUE)
split_cdb  

*SPLIT INTO A LIST OF* ContigCellDB() *BY NAMED FIELDS*

**Description**

Split into a list of *ContigCellDB()* by named fields

**Usage**

split_cdb(ccdb, fields, tbl = "contig_tbl", drop = FALSE, equalize = TRUE)

**Arguments**

- `ccdb` *ContigCellDB()*
- `fields` character naming fields in `tbl`
- `tbl` one of `contig_tbl`, `cell_tbl` or `cluster_tbl`
- `drop` logical indicating if levels that do not occur should be dropped (if *f* is a *factor* or a list).
- `equalize` logical. Should the contig, cells and clusters be equalized by taking the intersection of their common keys?

**Value**

list of *ContigCellDB*

**Examples**

```r
data(ccdb_ex)
splat = split_cdb(ccdb_ex, 'chain', 'contig_tbl')
stopifnot(all(splat$TRA$contig_tbl$chain == 'TRA'))
stopifnot(all(splat$TRB$contig_tbl$chain == 'TRB'))
```

**Description**

A *ContigCellDB* pretend to be a *cell_tbl* data.frame in several regards. This is to enable nesting *ContigCellDB* objects in the `cellData` of a `SingleCellExperiment` and so that various plotting functionality in `scater` can do something sensible.
Usage

## S4 method for signature 'ContigCellDB,character,missing'
x[[i, j, ...]]

## S4 method for signature 'ContigCellDB,ANY,missing,ANY'
x[i, j, ..., drop = TRUE]

## S4 method for signature 'ContigCellDB'
dim(x)

## S4 method for signature 'ContigCellDB'
dimnames(x)

## S4 method for signature 'ContigCellDB'
nrow(x)

## S4 method for signature 'ContigCellDB'
ncol(x)

Arguments

x  ContigCellDB
i  integer or character index
j  ignored
... ignored
drop ignored

Details

If x a ContigCellDB, then dim(x) and dimnames(x) return dim(x$cell_tbl) and dimnames(x$cell_tbl), respectively, and x[[col]] returns x$cell_tbl[[col]]. Likewise indexing with x[i,] returns cells indexed by i. Finally as.data.frame(x) returns x$cell_tbl.

Value

See details.

Examples

data(ccdb_ex)
ccdb_ex[1:10,]
head(ccdb_ex[['barcode']])
dim(ccdb_ex)
dimnames(ccdb_ex)
$ContigCellDB\text{-method}$

Access public members of ContigCellDB object.

Description

Modification to members will trigger various forms of equalization. See `equalize_ccdb()` for details.

Usage

```r
## S4 method for signature 'ContigCellDB'
x$name

## S4 replacement method for signature 'ContigCellDB'
x$name <- value
```

Arguments

- `x` A ContigCellDB object
- `name` a slot of a ContigCellDB object (one of `c('contig_tbl', 'cell_tbl', 'contig_pk', 'cell_pk', 'cluster_tbl', 'cluster_pk')`)
- `value` The value assigned to a slot of ContigCellDB object

Value

Update or return a slot of `ContigCellDB()`

See Also

`equalize_ccdb()`

Examples

```r
data(ccdb_ex)
ccdb_ex$contig_tbl
ccdb_ex$cell_tbl
ccdb_ex$cluster_tbl
data(ccdb_ex)
ccdb_ex$contig_pk = c("sample","barcode","contig_id") # 'pop' is technically redundant with 'sample'
# Take a subset of ccdb_ex
ccdb_ex
ccdb_ex$contig_tbl = dplyr::filter(ccdb_ex$contig_tbl, pop == 'b6')
ccdb_ex
```
# Index

## * datasets
- `ccdb_ex`, 7
- `contigs_qc`, 18
- `<cluster_permute_test`, 3
- `[,]ContigCellDB,ANY,missing,ANY-method
  ([[,]ContigCellDB,character,missing-method, 38
- `[,]ContigCellDB,ANY,missing-method
  ([[,]ContigCellDB,character,missing-method, 38
- `[[,]ContigCellDB,character,missing-method, 38
- `$,ContigCellDB-method, 40
- `$<-,ContigCellDB-method
  ($,ContigCellDB-method, 40
- Biostrings::stringDist(), 26
- canonicalize_cell, 4
- canonicalize_cell(), 6
- canonicalize_cluster, 5
- canonicalize_cluster(), 5
- ccdb.ex, 7
- ccdb_join, 7
- cdhit(), 9, 10
- cdhit(), 9
- cdhit_ccdb, 9
- cland, 10
- cluster_filterset, 11
- cluster_filterset(), 15
- cluster_germline, 12
- cluster_logistic_test
  (cluster_test_by), 15
- cluster_permute_test, 12
- cluster_permute_test(), 34
- cluster_plot, 14
- cluster_test_by, 15
- ContigCellDB, 16
- `ContigCellDB`) 4–6, 8–10, 12, 15, 17, 21, 23, 24, 26, 35, 36, 38, 40
- ContigCellDB-mutate
  (($.ContigCellDB-method), 40
- `ContigCellDB_10XVDJ (ContigCellDB), 16
- `contigs.qc, 7, 18
- `cross_tab_tbl, 19
- `methods.tab_by_celltype, 19
- crosstab_by_celltype(), 27
- `data.frame(), 29
- dim,ContigCellDB-method
  ([[,]ContigCellDB,character,missing-method), 38
- dimnames,ContigCellDB-method
  ([[,]ContigCellDB,character,missing-method), 38
- dplyr::filter(), 4, 6, 16, 23, 35
- dplyr::mutate(), 23
- entropy, 20
- enumerate_pairing(ig_chain_recode), 28
- equalize_ccdb, 21
- equalize_ccdb(), 40
- fancy_name_contigs, 22
- filter_cdb, 23
- filter_cdb(), 17
- fine_cluster_seqs, 24, 25
- fine_clustering, 24
- generate_pseudobulk, 26
- ggplot2::ggplot(), 29
- guess_celltype, 27
- guess_celltype(), 19
- hclust(), 26
- hushWarning, 27
- ig_chain_recode, 28
- left_join_warn (right_join_warn), 37
- left_join_warn(), 6
map_axis_labels, 29
modal_category (entropy), 20
mutate_cdb (filter_cdb), 23
mutate_cdb(), 17

col,ContigCellDB-method
   (c[[],ContigCellDB,character,missing-method), 38
np (entropy), 20
nrow,ContigCellDB-method
   (c[[],ContigCellDB,character,missing-method), 38

order(), 21

pairing_tables, 30
plot_cluster_factors, 32
plot_permute_test, 33
print.PermuteTest (plot_permute_test), 33
print.PermuteTestList
   (plot_permute_test), 33
purity, 34
purity(), 13

rank_chain_ccdb (rank_prevalence_ccdb), 34
rank_chain_ccdb(), 30
rank_prevalence_ccdb, 34
rank_prevalence_ccdb(), 30, 31
rbind,ContigCellDB-method, 36
rbind.ContigCellDB
   (rbind,ContigCellDB-method), 36
rbind.ContigCellDB(), 17
reexports, 36
right_join_warn, 37

split_cdb, 38
split_cdb(), 17

tcr_chain_recode (ig_chain_recode), 28
tibble::tibble(), 36, 37
tidy (reexports), 36
tidy.PermuteTest (plot_permute_test), 33
tidy.PermuteTestList
   (plot_permute_test), 33