# Package 'dowser'

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```
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Title B Cell Receptor Phylogenetics Toolkit
Description
     Provides a set of functions for inferring, visualizing, and analyzing B cell phylogenetic trees.
     Provides methods to 1) reconstruct unmutated ancestral sequences,
     2) build B cell phylogenetic trees using multiple methods,
     3) visualize trees with metadata at the tips,
     4) reconstruct intermediate sequences,
     5) detect biased ancestor-descendant relationships among metadata types
     Workflow examples available at documentation site (see URL).
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     Hoehn et al (2022) <doi:10.1371/journal.pcbi.1009885>,
     Hoehn et al (2021) <doi:10.1101/2021.01.06.425648>.
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```

Suggests knitr, rmarkdown, testthat, pwalign, BiocManager

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Type Package

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# Description

airrClone defines a common data structure for perform lineage reconstruction from AIRR data, based heavily on alakazam::ChangeoClone.

#### **Slots**

data data.frame containing sequences and annotations. Contains the columns sequence\_id and sequence, as well as any additional sequence-specific annotation columns

clone string defining the clone identifier

germline string containing the heavy chain germline sequence for the clone

lgermline string containing the light chain germline sequence for the clone

hlgermline string containing the combined germline sequence for the clone

v\_gene string defining the V segment gene call

j\_gene string defining the J segment gene call

junc\_len numeric junction length (nucleotide count)

locus index showing which locus represented at each site

region index showing FWR/CDR region for each site

phylo\_seq sequence column used for phylogenetic tree building

numbers index (usually IMGT) number of each site in phylo\_seq

### See Also

See formatClones for use.

BiopsyTrees 5

BiopsyTrees

Example Ig lineage trees with biopsy reconstructions.

# Description

Same as ExampleClones but with biopsies predicted at internal nodes

# Usage

BiopsyTrees

#### **Format**

A tibble of airrClone and phylo objects output by getTrees.

- clone\_id: Clonal cluster
- data: List of airrClone objects
- seqs: Number of sequences
- trees: List of phylo objects

# See Also

BiopsyTrees

bootstrapTrees

Deprecated! Please use findSwitches instead.

# Description

bootstrapTrees Phylogenetic bootstrap function.

# Usage

```
bootstrapTrees(
  clones,
  bootstraps,
  nproc = 1,
  trait = NULL,
  dir = NULL,
  id = NULL,
  modelfile = NULL,
  build = "pratchet",
  exec = NULL,
  igphyml = NULL,
  fixtrees = FALSE,
```

6 bootstrapTrees

```
quiet = 0,
rm_temp = TRUE,
palette = NULL,
resolve = 2,
rep = NULL,
keeptrees = TRUE,
lfile = NULL,
seq = NULL,
downsample = FALSE,
tip_switch = 20,
boot_part = "locus",
force_resolve = FALSE,
...
)
```

#### **Arguments**

clones tibble airrClone objects, the output of formatClones

number of bootstrap replicates to perform
nproc number of cores to parallelize computations

trait to use for parsimony models (required if igphyml specified)

dir directory where temporary files will be placed (required if igphyml or dnapars

specified)

id unique identifier for this analysis (required if igphyml or dnapars specified)

modelfile file specifying parsimony model to use

build program to use for tree building (phangorn, dnapars)

exec location of desired phylogenetic executable

igphyml location of igphyml executable if trait models desired

fixtrees keep tree topologies fixed? (bootstrapping will not be performed)

quiet amount of rubbish to print to console rm\_temp remove temporary files (default=TRUE)

palette deprecated

resolve how should polytomies be resolved? 0=none, 1=max parsimony, 2=max ambi-

guity + polytomy skipping, 3=max ambiguity

rep current bootstrap replicate (experimental)

keep trees estimated from bootstrap replicates? (TRUE)

lineage file input to igphyml if desired (experimental)

seq column name containing sequence information

downsample downsample clones to have a maximum specified tip/switch ratio?

tip\_switch maximum allowed tip/switch ratio if downsample=TRUE boot\_part is "locus" bootstrap columns for each locus separately

force\_resolve continue even if polytomy resolution fails?

additional arguments to be passed to tree building program

buildBeast 7

# Value

A list of trees and/or switch counts for each bootstrap replicate.

buildBeast

Read in a directory from a BEAST run. Runs treeannotator and log-analyser.

# **Description**

Read in a directory from a BEAST run. Runs treeannotator and loganalyser.

# Usage

```
buildBeast(
  data,
  beast,
  time,
  template,
  dir,
  id,
 mcmc_length = 1e+06,
  resume_clones = NULL,
  trait = NULL,
  asr = FALSE,
  full_posterior = FALSE,
  log_every = "auto",
  include_germline = TRUE,
  nproc = 1,
  quiet = 0,
  burnin = 10,
  low_ram = TRUE,
  germline_range = c(-10000, 10000),
  java = TRUE,
  seed = NULL,
  log_target = 10000,
  trees = NULL,
  tree_states = FALSE,
  start_edge_length = 100,
  start_date = NULL,
 max_start_date = NULL,
)
```

# **Arguments**

data

a list of airrClone objects

8 buildBeast

beast location of beast binary directory (beast/bin)

time Name of sample time column

template XML template

dir directory where temporary files will be placed.

id unique identifer for this analysis

mcmc\_length Number of MCMC steps

trait Trait column used

asr Log ancestral sequences?

full\_posterior Read un full distribution of parameters and trees?

log\_every Frequency of states logged. auto will divide mcmc\_length by log\_target

include\_germline

Include germline in analysis?

nproc Number of cores for parallelization. Uses at most 1 core per tree.

quiet Amount of rubbish to print to console

burnin Burnin percent (default 10)

low\_ram run with less memory (slightly slower)
germline\_range Possible date range of germline tip
java Use the -java flag for BEAST run

seed Use specified seeed for the -seed option for BEAST

trees optional list of starting trees, either phylo objects or newick strings

start\_edge\_length

edge length to use for all branches in starting tree

start\_date Starting date of time tree if desired

max\_start\_date Maximum starting date of time tree if desired

... Additional arguments for XML writing functions

#### Value

The input clones tibble with an additional column for the bootstrap replicate trees.

# See Also

getTimeTrees

buildClonalGermline 9

 $\begin{tabular}{ll} build Clonal Germline & Determine & consensus & clone & sequence & and & create & germline & for & clone \\ \end{tabular}$ 

# Description

Determine consensus clone sequence and create germline for clone

# Usage

```
buildClonalGermline(
  receptors,
  references,
  chain = "IGH",
  use_regions = FALSE,
  vonly = FALSE,
  seq = "sequence_alignment",
  id = "sequence_id",
  clone = "clone_id",
  v_call = "v_call",
  j_call = "j_call",
  j_germ_length = "j_germline_length",
  amino_acid = FALSE,
  ...
)
```

# Arguments

receptors	AIRR-table containing sequences from one clone
references	Full list of reference segments, see readIMGT
chain	chain in references being analyzed
use_regions	Return string of VDJ regions? (optional)
vonly	Return germline of only v segment?
seq	Column name for sequence alignment
id	Column name for sequence ID
clone	Column name for clone ID
v_call	Column name for V gene segment gene call
j_call	Column name for J gene segment gene call
j_germ_length	Column name of J segment length within germline
j_germ_aa_length	
	Column name of J segment amino acid length (if amino_acid=TRUE)
amino_acid	Perform reconstruction on amino acid sequence (experimental)
	Additional arguments passed to buildGermline

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#### **Details**

Return object adds/edits following columns:

- seq: Sequences potentially padded same length as germline
- germline\_alignment: Full length germline
- germline\_alignment\_d\_mask: Full length, D region masked
- vonly: V gene segment of germline if vonly=TRUE
- regions: String of VDJ segment in position if use\_regions=TRUE

#### Value

Tibble with reconstructed germlines

#### See Also

createGermlines buildGermline, stitchVDJ

buildGermline

buildGermline reconstruct germline segments from alignment data

# **Description**

Reconstruct germlines from alignment data.

# Usage

```
buildGermline(
  receptor.
  references,
  seq = "sequence_alignment",
  id = "sequence_id",
  clone = "clone_id",
  v_call = "v_call",
  d_call = "d_call",
  j_call = "j_call",
  v_germ_start = "v_germline_start",
  v_germ_end = "v_germline_end",
  v_germ_length = "v_germline_length",
  d_germ_start = "d_germline_start",
  d_germ_end = "d_germline_end",
  d_germ_length = "d_germline_length",
  j_germ_start = "j_germline_start",
  j_germ_end = "j_germline_end",
  j_germ_length = "j_germline_length",
  np1_length = "np1_length",
  np2_length = "np2_length",
  amino_acid = FALSE
)
```

buildGermline 11

# Arguments

receptor	row from AIRR-table containing sequence of interest
references	list of reference segments. Must be specific to locus
seq	Column name for sequence alignment
id	Column name for sequence ID
clone	Column name for clone ID
v_call	Column name for V gene segment gene call
d_call	Column name for D gene segment gene call
j_call	Column name for J gene segment gene call
v_germ_start	Column name of index of V segment start within germline
v_germ_end	Column name of index of V segment end within germline
v_germ_length	Column name of index of V segment length within germline
d_germ_start	Column name of index of D segment start within germline
d_germ_end	Column name of index of D segment end within germline
d_germ_length	Column name of index of D segment length within germline
j_germ_start	Column name of index of J segment start within germline
j_germ_end	Column name of index of J segment end within germline
j_germ_length	Column name of index of J segment length within germline
np1_length	Column name in receptor specifying np1 segment length
np2_length	Column name in receptor specifying np2 segment length
amino_acid	Perform reconstruction on amino acid sequence (experimental)

# **Details**

Return object contains multiple IMGT-gapped germlines:

- full: Full length germline
- dmask: Full length germline with D region masked
- vonly: V gene segment of germline
- regions: String showing VDJ segment of each position

# Value

List of reconstructed germlines

# See Also

buildClonalGermline, stitchVDJ

buildIgphyml

buildIgphyml

Wrapper to build IgPhyML trees and infer intermediate nodes

# Description

Wrapper to build IgPhyML trees and infer intermediate nodes

# Usage

```
buildIgphyml(
  clone,
  igphyml,
  trees = NULL,
  nproc = 1,
  temp_path = NULL,
  id = NULL,
  rseed = NULL,
  quiet = 0,
  rm_files = TRUE,
  rm_dir = NULL,
  partition = c("single", "cf", "hl", "hlf", "hlc", "hlcf"),
  omega = NULL,
  optimize = "lr",
  motifs = "FCH",
  hotness = "e,e,e,e,e,e",
  rates = NULL,
  asrc = 0.95,
  splitfreqs = FALSE,
  asrp = FALSE,
  make_gyrep = TRUE,
)
```

# **Arguments**

clone	list of airrClone objects
igphyml	igphyml executable
trees	list of tree topologies if desired
nproc	number of cores for parallelization
temp_path	path to temporary directory
id	IgPhyML run id
rseed	random number seed if desired
quiet	amount of rubbish to print
rm_files	remove temporary files?

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rm\_dir remove temporary directory?

partition How to partition omegas along sequences (see details)
omega omega parameters to estimate (see IgPhyML docs)
optimize optimize HLP rates (r), lengths (l), topology (t)

motifs motifs to consider (see IgPhyML docs)

hotness hotness parameters to estimate (see IgPhyML docs)

rates comma delimited list showing which omega-defined partitions get a separate

rate (e.g. omega=e,e rates=0,1).

asrc Intermediate sequence cutoff probability

splitfreqs Calculate codon frequencies on each partition separately?

asrp Run ASRp?

make\_gyrep Create the grep file?

... Additional arguments (not currently used)

### **Details**

Partition options in rate order:

• single: 1 omega for whole sequence

• cf: 2 omegas, 1 for all CDRs and 1 for all FWRs

• h1: 2 omegas, 1 for heavy and 1 for light chain

• hlf: 3 omegas, 1 for heavy FWR, 1 for all CDRs, and 1 for light FWRs

• hlc: 3 omegas, 1 for all FWRs, 1 for heavy CDRs, and 1 for light CDRs

• hlcf: 4 omegas, 1 for each heavy FWR, 1 for heavy CDR, 1 for light FWR, and 1 for light CDR

#### Value

phylo object created by igphyml with nodes attribute containing reconstructed sequences.

buildPhylo Wrapper for alakazam::buildPhylipLineage

#### **Description**

Wrapper for alakazam::buildPhylipLineage

14 buildPML

#### Usage

```
buildPhylo(
  clone,
  exec,
  temp_path = NULL,
  verbose = 0,
  rm_temp = TRUE,
  seq = "sequence",
  tree = NULL,
  onetree = TRUE
)
```

#### **Arguments**

clone airrClone object dnapars or dnaml executable exec path to temporary directory temp\_path verbose amount of rubbish to print remove temporary files? rm\_temp sequence column in airrClone object seq fixed tree topology if desired (currently does nothing if specified) tree onetree Only sample one tree if multiple found.

# Value

phylo object created by dnapars or dnaml with nodes attribute containing reconstructed sequences.

buildPML

Wrapper for phangorn::optim.pml

# **Description**

Wrapper for phangorn::optim.pml

# Usage

```
buildPML(
  clone,
  seq = "sequence",
  sub_model = "GTR",
  gamma = FALSE,
  asr = "seq",
  asr_thresh = 0.05,
  tree = NULL,
  data_type = "DNA",
```

buildPML 15

```
optNni = TRUE,
optQ = TRUE,
optEdge = TRUE,
verbose = FALSE,
resolve_random = TRUE,
quiet = 0,
rep = NULL,
dir = NULL,
id = NULL,
asrp = FALSE
)
```

# Arguments

clone airrClone object

seq sequence column in airrClone object

sub\_model substitution model to use gamma gamma site rate variation?

asr return sequence or probability matrix?

asr\_thresh threshold for including a nucleotide as an alternative

tree fixed tree topology if desired.
data\_type Are sequences DNA or AA?

optNni Optimize tree topology
optQ Optimize Q matrix
optEdge Optimize edge lengths

verbose Print error messages as they happen?

resolve\_random randomly resolve polytomies?

quiet amount of rubbish to print to console
rep current bootstrap replicate (experimental)

dir A directory to save the codon table

id The identifier value asrp Get the codon table?

### Value

phylo object created by phangorn::optim.pml with nodes attribute containing reconstructed sequences.

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buildPratchet

Wrapper for phangorn::pratchet

# Description

Wrapper for phangorn::pratchet

# Usage

```
buildPratchet(
  clone,
  seq = "sequence",
  asr = "seq",
  asr_thresh = 0.05,
  tree = NULL,
  asr_type = "MPR",
  verbose = 0,
  resolve_random = TRUE,
  data_type = "DNA"
)
```

# Arguments

clone	airrClone object
seq	sequence column in airrClone object
asr	return sequence or probability matrix?
asr_thresh	threshold for including a nucleotide as an alternative
tree	fixed tree topology if desired.
asr_type	MPR or ACCTRAN
verbose	amount of rubbish to print
resolve_random	randomly resolve polytomies?
data_type	Are sequences DNA or AA?

# Value

phylo object created by phangorn::pratchet with nodes attribute containing reconstructed sequences.

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buildRAxML

Wrapper to build RAxML-ng trees and infer intermediate nodes

# Description

Wrapper to build RAxML-ng trees and infer intermediate nodes

# Usage

```
buildRAxML(
  clone,
  exec,
  seq = "sequence",
  sub_model = "GTR",
  partition = NULL,
  rseed = 28,
  name = "run",
  starting_tree = NULL,
  data_type = "DNA",
  from_getTrees = FALSE,
  rm_files = TRUE,
  asr = TRUE,
  rep = 1,
 dir = NULL,
  n_starts = NULL,
)
```

# **Arguments**

clone	list of airrClone objects
exec	RAxML-ng executable
seq	the phylo_seq option does this clone uses. Possible options are "sequence", "hlsequence", or "lsequence"
sub_model	The DNA model to be used. GTR is the default.
partition	A parameter that determines how branches are reported when partitioning. Options include NULL (default), scaled, unlinked, and linked
rseed	The random seed used for the parsimony inferences. This allows you to reproduce your results.
name	specifies the name of the output file
starting_tree	specifies a user starting tree file name and path in Newick format
data_type	Specifies what format your data is in, DNA or AA
<pre>from_getTrees</pre>	A logical that indicates if the desired starting tree is from getTrees and not a newick file

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rm_files	remove temporary files?
asr	computes the marginal ancestral states of a tree
rep	Which repetition of the tree building is currently being run. Mainly for getBootstraps.
dir	Where the output files are to be made.
n_starts	Number of max parsimony starting trees (default is 10 pars + 10 random)
	Additional arguments (not currently used)

# Value

phylo object created by RAxML-ng with nodes attribute containing reconstructed sequences.

calcRF	Finds the Robinson-Fould's cluster distance between phylogenies.

# Description

calcRF Calculates the RF distance between two phylogenetic trees with the same tips and tip labels.

# Usage

```
calcRF(tree_1, tree_2, nproc = 1)
```

# Arguments

tree_1	A phylo object
tree_2	A phylo object
nproc	Number of cores to use for calculations.

# Value

The RF cluster value for the two input trees.

checkDivergence 19

checkDivergence	Compare divergence along a tree in terms of mutations (sum of
	branches) for each tip and reconstructed internal node to its Ham-
	ming distance from the germline. Divergence should never be less than Hamming distance. A threshold of -1 is used to represent 1 full
	mutation difference. The function will throw a warning if any trees
	cross this threshold

# Description

Compare divergence along a tree in terms of mutations (sum of branches) for each tip and reconstructed internal node to its Hamming distance from the germline. Divergence should never be less than Hamming distance. A threshold of -1 is used to represent 1 full mutation difference. The function will throw a warning if any trees cross this threshold

# Usage

```
checkDivergence(
  clones,
  threshold = -1,
  verbose = TRUE,
  germline = "Germline",
  data_type = "DNA"
)
```

# Arguments

clones	a tibble of clones and trees, output from getTrees	
threshold	shold Minimum allowed value of divergence minus Hamming distant	
verbose	Print whether all trees passed	
germline	ID of the tree's predicted germline sequence	
data_type	The type of data being used. Either "DNA" (default) or "AA"	

#### Value

tibble showing the clone\_id, sequence\_id, as well as tree-based divergence, hamming distance, and difference between the two.

20 colorTrees

collapseNodes

Collapse internal nodes with the same predicted sequence

### **Description**

collapseNodes Node collapsing function.

# Usage

```
collapseNodes(trees, tips = FALSE, check = TRUE)
```

# **Arguments**

trees a tibble of airrClone objects, the output of getTrees

tips collapse tips to internal nodes? (experimental)

check check that collapsed nodes are consistent with original tree

#### **Details**

Use plotTrees(trees)[[1]] + geom\_label(aes(label=node)) + geom\_tippoint() to show node labels, and getSeq to return internal node sequences

#### Value

A tibble with phylo objects that have had internal nodes collapsed.

### See Also

getTrees

colorTrees

Get a color palette for a predefined set of trait values

### **Description**

colorTree Gets a color palette for a predefined set of trait values

# Usage

```
colorTrees(trees, palette, ambig = "blend")
```

### **Arguments**

trees list of phylo objects with assigned internal node states

palette named vector of colors (see getPalette)

ambig how should ambiguous states be colored (blend or grey)

condenseTrees 21

# **Details**

Trees must have node states represented in a "states" vector. By default, ambiguous states (separated by ",") have their colors blended. If

# Value

A list of colored trees

#### See Also

getPalette, getTrees, plotTrees

 $condense {\sf Trees}$ 

Condense a set of equally parsimonious node labels into a single tree

# Description

condenseTrees Condenses a set of equally parsimonious node labels into a single tree

# Usage

```
condenseTrees(trees, states, palette = NULL)
```

# **Arguments**

trees List of the same tree with equally parsimonious labels

states States in model

palette Named vector with a color per state

#### Value

a phylo object representing all represented internal node states

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correlationTest

Run date randomization test for temporal signal on a set of trees.

#### **Description**

correlationTest performs root-to-tip regression date randomization test

#### Usage

```
correlationTest(
  clones,
  permutations = 1000,
  minlength = 0.001,
  perm_type = c("clustered", "uniform"),
  time = "time",
  sequence = "sequence_id",
  germline = "Germline",
  verbose = FALSE,
  polyresolve = TRUE,
  alternative = c("greater", "two.sided"),
  storeTree = FALSE,
  nproc = 1
)
```

# **Arguments**

clones	A tibble object containing airrClone and phylo objects
permutations	Number of permutations to run

minlength Branch lengths to collapse in trees

perm\_type Permute among single timepoint clades or uniformly among tips

time Column name holding numeric time information

sequence Column name holding sequence ID

germline Germline sequence name

verbose Print lots of rubbish while running?

polyresolve Resolve polytomies to have a minimum number of single timepoint clades

alternative Is alternative that the randomized correlation are greater than or equal to ob-

served, or greater/less than?

storeTree Store the tree used?

nproc Number of cores to use for calculations. Parallelizes by tree.

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#### **Details**

Object returned contains these columns which are added or modified from input:

• data: airrClone object, same as input but with additional columns "cluster" which correspond to permutation cluster, and "divergence."

- slope: Slope of linear regression between divergence and time.
- correlation: Correlation between divergence and time.
- p: p value of correlation compared to permuted correlations.
- random\_correlation: Mean correlation of permutation replicates.
- min\_p: Minimum p value of data, determined by either the number of distinct clade/timepoint combinations or number of permutations.
- nposs: Number of possible distinct timepoint/clade combinations.
- nclust: Number of clusters used in permutation. If perm\_type="uniform" this is the number of tips.
- p\_gt/p\_lt: P value that permuted correlations are greater or less than observed correlation. Only returned if alternative = "two.sided"
- test\_trees: The phylo tree objects used, possibly with resolved polytomies.

#### Value

A tibble with the same columns as clones, but additional columns corresponding to test statistics for each clone.

#### See Also

Uses output from getTrees.

createGermlines

createGermlines Determine consensus clone sequence and create germline for clone

### **Description**

createGermlines Determine consensus clone sequence and create germline for clone

# Usage

```
createGermlines(
  data,
  references,
  locus = "locus",
  trim_lengths = FALSE,
  force_trim = FALSE,
  nproc = 1,
```

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```
seq = "sequence_alignment",
  v_call = "v_call",
 d_call = "d_call",
  j_call = "j_call",
  amino_acid = FALSE,
  id = "sequence_id",
  clone = "clone_id",
  v_germ_start = "v_germline_start",
  v_germ_end = "v_germline_end",
  v_germ_length = "v_germline_length",
 d_germ_start = "d_germline_start",
 d_germ_end = "d_germline_end",
 d_germ_length = "d_germline_length",
  j_germ_start = "j_germline_start",
  j_germ_end = "j_germline_end",
  j_germ_length = "j_germline_length",
 np1_length = "np1_length",
 np2_length = "np2_length",
 na.rm = TRUE,
  fields = NULL,
 verbose = 0,
)
```

# Arguments

data	AIRR-table containing sequences from one clone	
references	Full list of reference segments, see readIMGT	
locus	Name of the locus column in the input data	
trim_lengths	Remove trailing Ns from seq column if length different from germline?	
force_trim	Remove all characters from sequence if different from germline? (not recommended)	
nproc	Number of cores to use	
seq	Column name for sequence alignment	
v_call	Column name for V gene segment gene call	
d_call	Column name for D gene segment gene call	
j_call	Column name for J gene segment gene call	
amino_acid	Perform reconstruction on amino acid sequence (experimental)	
id	Column name for sequence ID	
clone	Column name for clone ID	
v_germ_start	Column name of index of V segment start within germline	
v_germ_end	Column name of index of V segment end within germline	
v_germ_length	Column name of index of V segment length within germline	
d_germ_start	Column name of index of D segment start within germline	

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d_germ_end	Column name of index of D segment end within germline
d_germ_length	Column name of index of D segment length within germline
j_germ_start	Column name of index of J segment start within germline
j_germ_end	Column name of index of J segment end within germline
j_germ_length	Column name of index of J segment length within germline
np1_length	Column name in receptor specifying np1 segment length
np2_length	Column name in receptor specifying np2 segment length
na.rm	Remove clones with failed germline reconstruction?
fields	Character vector of additional columns to use for grouping. Sequences with disjoint values in the specified fields will be considered as separate clones.
verbose	amount of rubbish to print
	Additional arguments passed to buildGermline

#### **Details**

Return object adds/edits following columns:

- seq: Sequences potentially padded same length as germline
- germline\_alignment: Full length germline
- germline\_alignment\_d\_mask: Full length, D region masked
- vonly: V gene segment of germline if vonly=TRUE
- regions: String of VDJ segment in position if use\_regions=TRUE

# Value

Tibble with reconstructed germlines

#### See Also

createGermlines buildGermline, stitchVDJ

# Examples

```
vdj_dir <- system.file("extdata", "germlines", "imgt", "human", "vdj", package="dowser")
imgt <- readIMGT(vdj_dir)
db <- createGermlines(ExampleAirr[1,], imgt)</pre>
```

26 create\_height\_prior

# **Description**

Takes an airr clone object and returns BEAST2 Alignment xml of the sequences

#### Usage

```
create_alignment(clone, id, include_germline_as_tip)
```

# Arguments

clone an airrClone object

id unique identifer for this analysis

include\_germline\_as\_tip

include the germline as a tip in the alignment?

#### Value

String of BEAST2 Alignment and TaxonSet xml

#### **Description**

Takes an airr clone object and returns BEAST2 XML to set a height prior

# Usage

```
create_height_prior(clone, id, start_date)
```

#### **Arguments**

clone an airrClone object

id unique identifer for this analysis

start\_date starting date to use as prior, in forward time

# Value

String of XML setting the height prior

create\_max\_height\_prior

Takes an airr clone object and returns BEAST2 XML to set a maximum height prior

# **Description**

Takes an airr clone object and returns BEAST2 XML to set a maximum height prior

# Usage

```
create_max_height_prior(clone, id, max_start_date)
```

### **Arguments**

clone an airrClone object

id unique identifer for this analysis

max\_start\_date max start date to use for prior, in forward time

#### Value

String of XML setting the MRCA prior of the observed sequences

```
create_MRCA_prior_germline
```

Takes an airr clone object and returns BEAST2 XML for MRCA prior of the germline sequence

# **Description**

Takes an airr clone object and returns BEAST2 XML for MRCA prior of the germline sequence

# Usage

```
create_MRCA_prior_germline(clone, id, germline_range)
```

#### **Arguments**

clone an airrClone object

id unique identifer for this analysis germline\_range Possible date range of germline tip

### Value

String of XML setting the MRCA prior of the germline sequence

28 create\_root\_freqs

create\_MRCA\_prior\_observed

Takes an airr clone object and returns BEAST2 XML for MRCA prior of the observed sequences

# **Description**

Takes an airr clone object and returns BEAST2 XML for MRCA prior of the observed sequences

# Usage

```
create_MRCA_prior_observed(clone, id)
```

# Arguments

clone an airrClone object

id unique identifer for this analysis

#### Value

String of XML setting the MRCA prior of the observed sequences

create\_root\_freqs

Takes an airr clone object and returns BEAST2 rootfreqs xml of the germline

# **Description**

Takes an airr clone object and returns BEAST2 rootfreqs xml of the germline

# Usage

```
create_root_freqs(clone, id)
```

### **Arguments**

clone an airrClone object

id unique identifer for this analysis

# Value

String of XML setting the root frequencies to the germline sequence

create\_starting\_tree 29

#### **Description**

Takes an airr clone object and tree and returns BEAST2 XML for setting the starting tree

# Usage

```
create_starting_tree(
  clone,
  id,
  tree,
  include_germline_as_tip,
  tree_states,
  start_edge_length
)
```

# **Arguments**

```
clone an airrClone object

id unique identifer for this analysis

tree starting tree, either a phylo object or a newick string

include_germline_as_tip

include the germline as a tip

tree_states use states in the starting tree?

start_edge_length

edge length to use for all branches in starting tree
```

### Value

String of XML setting the starting tree

# **Description**

Takes an airr clone object and returns BEAST2 XML for a trait/traitSet from a column

30 dfToFasta

#### Usage

```
create_traitset(
  clone,
  trait_name,
  column,
  id,
  trait_data_type = NULL,
  isSet = FALSE,
  include_germline_as_tip = FALSE
)
```

# **Arguments**

# Value

String of XML of the trait or traitSet

dfToFasta

Write a fasta file of sequences readFasta reads a fasta file

# Description

Write a fasta file of sequences readFasta reads a fasta file

# Usage

```
dfToFasta(
   df,
   file,
   id = "sequence_id",
   seq = "sequence",
   imgt_gaps = FALSE,
   columns = NULL
)
```

downsampleClone 31

### **Arguments**

df	dataframe of sequences
file	FASTA file for output

id Column name of sequence ids
seq Column name of sequences
imgt\_gaps Keep IMGT gaps if present?

columns vector of column names to append to sequence id

#### Value

File of FASTA formatted sequences

downsampleClone

downsampleClone Down-sample clone to maximum tip/switch ratio

# **Description**

downsampleClone Down-sample clone to maximum tip/switch ratio

# Usage

```
downsampleClone(clone, trait, tip_switch = 20, tree = NULL)
```

# Arguments

clone an airrClone object

trait trait considered for rarefaction getTrees

tip\_switch maximum tip/switch ratio

tree a phylo tree object correspond to clone

# Value

A vector with sequence for each locus at a specified node in tree.

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dowser

The dowser package

# **Description**

dowser is a phylogenetic analysis package as part of the Immcantation suite of tools. For additional details regarding the use of the dowser package see the vignettes: browseVignettes("dowser")

#### References

1. Hoehn KB, Pybus OG, Kleinstein SH (2022) Phylogenetic analysis of migration, differentiation, and class switching in B cells. PLoS Computational Biology. https://doi.org/10.1371/journal.pcbi.1009885

ExampleAirr

Example AIRR database

# **Description**

A small example database subset from Laserson and Vigneault et al, 2014.

#### Usage

ExampleAirr

#### **Format**

A data.frame with the following AIRR style columns:

- sequence\_id: Sequence identifier
- sequence\_alignment: IMGT-gapped observed sequence.
- germline\_alignment\_d\_mask: IMGT-gapped germline sequence with N, P and D regions masked.
- v\_call: V region allele assignments.
- v\_call\_genotyped: TIgGER corrected V region allele assignment.
- d\_call: D region allele assignments.
- j\_call: J region allele assignments.
- junction: Junction region sequence.
- junction\_length: Length of the junction region in nucleotides.
- np1\_length: Combined length of the N and P regions proximal to the V region.
- np2\_length: Combined length of the N and P regions proximal to the J region.
- sample: Sample identifier. Time in relation to vaccination.
- isotype: Isotype assignment.
- duplicate\_count: Copy count (number of duplicates) of the sequence.
- clone\_id: Change-O assignment clonal group identifier.

ExampleAirrTyCHE 33

#### References

1. Laserson U and Vigneault F, et al. High-resolution antibody dynamics of vaccine-induced immune responses. Proc Natl Acad Sci USA. 2014 111:4928-33.

# See Also

ExampleDbChangeo ExampleClones

ExampleAirrTyCHE

Example AIRR database for TyCHE

# **Description**

A small example database from simble.

### Usage

ExampleAirrTyCHE

#### **Format**

A data.frame with the following AIRR style columns:

- sequence\_id: Sequence identifier
- sequence\_alignment: IMGT-gapped observed sequence.
- germline\_alignment: IMGT-gapped germline sequence.
- v\_call: V region allele assignments.
- d\_call: D region allele assignments.
- j\_call: J region allele assignments.
- junction: Junction region sequence.
- junction\_length: Length of the junction region in nucleotides.
- np1\_length: Combined length of the N and P regions proximal to the V region.
- np2\_length: Combined length of the N and P regions proximal to the J region.
- sample\_time: Time point of the sample.
- location: Location of tissue from which the sample was taken.
- clone\_id: Clonal group identifier.

# References

1. Pre-submission.

34 ExampleDbChangeo

ExampleClones

Example Ig lineage trees

# **Description**

A tibble of Ig lineage trees generated from the ExampleAirr file

# Usage

ExampleClones

#### **Format**

A tibble of airrClone and phylo objects output by getTrees.

- clone\_id: Clonal cluster
- data: List of airrClone objects
- seqs: Number of sequences
- trees: List of phylo objects

# See Also

ExampleClones

ExampleDbChangeo

Example Change-O database

# Description

A small example database subset from Laserson and Vigneault et al, 2014.

# Usage

ExampleDbChangeo

# **Format**

A data.frame with the following Change-O style columns:

- SEQUENCE\_ID: Sequence identifier
- SEQUENCE\_IMGT: IMGT-gapped observed sequence.
- GERMLINE\_IMGT\_D\_MASK: IMGT-gapped germline sequence with N, P and D regions masked.
- V\_CALL: V region allele assignments.
- V\_CALL\_GENOTYPED: TIgGER corrected V region allele assignment.

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- D\_CALL: D region allele assignments.
- J\_CALL: J region allele assignments.
- JUNCTION: Junction region sequence.
- JUNCTION\_LENGTH: Length of the junction region in nucleotides.
- NP1\_LENGTH: Combined length of the N and P regions proximal to the V region.
- NP2\_LENGTH: Combined length of the N and P regions proximal to the J region.
- SAMPLE: Sample identifier. Time in relation to vaccination.
- ISOTYPE: Isotype assignment.
- DUPCOUNT: Copy count (number of duplicates) of the sequence.
- CLONE: Change-O assignment clonal group identifier.

#### References

1. Laserson U and Vigneault F, et al. High-resolution antibody dynamics of vaccine-induced immune responses. Proc Natl Acad Sci USA. 2014 111:4928-33.

#### See Also

ExampleAirr ExampleClones

ExampleMixedClones

Example Multiple Partition Trees

# Description

A small example database subset from Turner, J. S. et al. Human germinal centres engage memory and naive B cells after influenza vaccination. Nature 586, 127–132 (2020).

### Usage

ExampleMixedClones

#### **Format**

A data.frame with the following Change-O style columns:

- clone\_id: Clonal cluster
- data: List of airrClone objects
- locus: Locus identifier.
- seqs: Number of sequences
- igphyml\_partitioned\_trees: IgPhyML partitioned tree
- raxml\_partitioned\_trees: RAxML partitioned tree

36 ExampleMixedDb

ExampleMixedDb

Example Change-O database

#### **Description**

A small example database subset from Turner, J. S. et al. Human germinal centres engage memory and naive B cells after influenza vaccination. Nature 586, 127–132 (2020).

#### Usage

ExampleMixedDb

#### **Format**

A data.frame with the following Change-O style columns:

- sequence\_id: Sequence identifier
- sequence: B cell sequence
- productive: A logical indicating if the sequence is productive.
- v\_call: V region allele assignments.
- d\_call: D region allele assignments.
- j\_call: J region allele assignments.
- sequence\_alignment: Sequence alignment.
- germline\_alignment: Germline alignment without gaps.
- junction: Junction
- juncation\_aa: Junction aa
- vj\_inframe: A logical to see if the vj genes are in frame
- stop\_codon: A indicator if there is a stop codon within the alignment
- locus: Locus identifier.
- ullet v\_sequence\_start: Where the V gene starts
- v\_sequence\_end: Where the V gene ends
- v\_germline\_start: Where the V germline starts
- v\_germline\_end: Where the V germline ends
- np1\_length: Length of np1
- d\_sequence\_start: Where the D gene starts
- d\_sequence\_end: Where the D gene ends
- d\_germline\_start: Where the D germline starts
- d\_germline\_end: Where the D germline ends
- np2\_length: Length of np2
- j\_sequence\_start: Where the J gene starts

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- j\_sequence\_end: Where the J gene ends
- j\_germline\_start: Where the J germline starts
- j\_germline\_end: Where the J germline ends
- junction\_length: Length of the junction region in nucleotides.
- v\_score: V score
- v\_identity: Identity score of V
- v\_support: V support
- d\_score: D score
- d\_identity: D identity
- d\_support: D support
- j\_score: J score
- j\_support: J support
- j\_identity: J identity
- cell\_id: Cell identifier
- consensus\_count: Consensus count
- indels: Logical if indels are present
- sequence\_vdj: VDJ sequence
- v\_germ\_start\_vdj: Where the V germline starts on the VDJ
- v\_germ\_end\_vdj: Where the V germline ends on the VDJ
- subject: Subject identifier
- timepoint: Day the sample was taken
- cell\_type: Type of cell
- replicate: Replicate number
- clone\_id: Change-O assignment clonal group identifier.
- seq\_type: Identifier of data type (10x)
- vj\_gene: VJ gene
- vj\_alt\_gene: Alternative VJ gene
- v\_germline\_length: Length of the V germline segment
- $\bullet$  d\_germline\_length: Length of the D germline segment
- j\_germline\_lenght: Length of the J germline segment
- germline\_alignment\_d\_mask: Germline alignment with gaps

38 findSwitches

exportTrees

Exports the phylogenetic trees from the airrClone object

## Description

```
exportTrees Exports phylogenetic trees
```

## Usage

```
exportTrees(clones, filepath, tree_column = "trees", ...)
```

## **Arguments**

clones tibble airrClone objects, the output of formatClones

filepath The file path for where the trees will be saved tree\_column The name of the column that contains the trees

... additional arguments to be passed

findSwitches

Create a bootstrap distribution for clone sequence alignments, and

estimate trees for each bootstrap replicate.

## **Description**

findSwitches Phylogenetic bootstrap function.

```
findSwitches(
  clones,
  permutations,
  trait,
  igphyml,
  fixtrees = FALSE,
  downsample = TRUE,
  tip_switch = 20,
  nproc = 1,
  dir = NULL,
  id = NULL,
 modelfile = NULL,
 build = "pratchet",
  exec = NULL,
  quiet = 0,
  rm_temp = TRUE,
```

findSwitches 39

```
palette = NULL,
resolve = 2,
rep = NULL,
keeptrees = FALSE,
lfile = NULL,
seq = NULL,
boot_part = "locus",
force_resolve = FALSE,
...
)
```

## Arguments

clones tibble airrClone objects, the output of formatClones

permutations number of bootstrap replicates to perform

trait trait to use for parsimony models igphyml location of igphyml executable

fixtrees keep tree topologies fixed? (bootstrapping will not be performed)
downsample downsample clones to have a maximum specified tip/switch ratio?

tip\_switch maximum allowed tip/switch ratio if downsample=TRUE

nproc number of cores to parallelize computations

dir directory where temporary files will be placed (required if igphyml or dnapars

specified)

id unique identifier for this analysis (required if igphyml or dnapars specified)

modelfile file specifying parsimony model to use

build program to use for tree building (phangorn, dnapars)

exec location of desired phylogenetic executable

quiet amount of rubbish to print to console rm\_temp remove temporary files (default=TRUE)

palette deprecated

resolve how should polytomies be resolved? 0=none, 1=max parsimony, 2=max ambi-

guity + polytomy skipping, 3=max ambiguity

rep current bootstrap replicate (experimental)

keeptrees keep trees estimated from bootstrap replicates? (TRUE)

lineage file input to igphyml if desired (experimental)

seq column name containing sequence information

boot\_part is "locus" bootstrap columns for each locus separately

force\_resolve continue even if polytomy resolution fails?

additional arguments to be passed to tree building program

40 formatClones

#### **Details**

Tree building details are the same as getTrees. If keeptrees=TRUE (default) the returned object will contain a list named "trees" which contains a list of estimated tree objects for each bootstrap replicate. The object is structured like: trees[[<replicate>]][[<tree index>]]. If igphyml is specified (as well as trait), the returned object will contain a tibble named "switches" containing switch count information. This object can be passed to testSP and other functions to perform parsimony based trait value tests.

Trait values cannot contain values N, UCA, or NTIP. These are reserved for use by test statistic functions.

#### Value

A list of trees and/or switch counts for each bootstrap replicate.

### See Also

Uses output from formatClones with similar arguments to getTrees. Output can be visualized with plotTrees, and tested with testPS, testSC, and testSP.

### **Examples**

```
## Not run:
data(ExampleAirr)
ExampleAirr$sample_id <- sample(ExampleAirr$sample_id)
clones <- formatClones(ExampleAirr, trait="sample_id")

igphyml <- "~/apps/igphyml/src/igphyml"
btrees <- findSwitches(clones[1:2,], permutations=10, nproc=1, igphyml=igphyml, trait="sample_id")
plotTrees(btrees$trees[[4]])[[1]]
testPS(btrees$switches)

## End(Not run)</pre>
```

formatClones

Generate an ordered list of airrClone objects for lineage construction

### **Description**

formatClones takes a data. frame or tibble with AIRR or Change-O style columns as input and masks gap positions, masks ragged ends, removes duplicates sequences, and merges annotations associated with duplicate sequences. If specified, it will un-merge duplicate sequences with different values specified in the traits option. It returns a list of airrClone objects ordered by number of sequences which serve as input for lineage reconstruction.

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## Usage

```
formatClones(
  data,
  seq = "sequence_alignment",
 clone = "clone_id",
  subgroup = "clone_subgroup",
  id = "sequence_id",
  germ = "germline_alignment_d_mask",
  v_call = "v_call",
  j_call = "j_call",
  junc_len = "junction_length",
 mask_char = "N",
 max_mask = 0,
 pad_end = TRUE,
  text_fields = NULL,
  num_fields = NULL,
  seq_fields = NULL,
  add_count = TRUE,
  verbose = FALSE,
  collapse = TRUE,
  cell = "cell_id",
 locus = "locus",
  traits = NULL,
 mod3 = TRUE,
 randomize = TRUE,
  use_regions = TRUE,
  dup_singles = FALSE,
  nproc = 1,
  chain = "H",
  heavy = "IGH",
  filterstop = TRUE,
 minseq = 2,
  split_light = FALSE,
  light_traits = FALSE,
 majoronly = FALSE,
  columns = NULL
)
```

# Arguments

data	data.frame containing the AIRR or Change-O data for a clone. See makeAirrClone for required columns and their defaults
seq	name of the column containing observed DNA sequences. All sequences in this column must be multiple aligned.
clone	name of the column containing the identifier for the clone. All entries in this column should be identical.
subgroup	name of the column containing the identifier for the subgroup.

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id name of the column containing sequence identifiers. germ name of the column containing germline DNA sequences. All entries in this column should be identical for any given clone, and they must be multiple aligned with the data in the seq column. v\_call name of the column containing V-segment allele assignments. All entries in this column should be identical to the gene level. name of the column containing J-segment allele assignments. All entries in this j\_call column should be identical to the gene level. name of the column containing the length of the junction as a numeric value. junc\_len All entries in this column should be identical for any given clone. mask\_char character to use for masking and padding. maximum number of characters to mask at the leading and trailing sequence max\_mask ends. If NULL then the upper masking bound will be automatically determined from the maximum number of observed leading or trailing Ns amongst all sequences. If set to 0 (default) then masking will not be performed. if TRUE pad the end of each sequence with mask\_char to make every sequence pad\_end the same length. text annotation columns to retain and merge during duplicate removal. text fields num\_fields numeric annotation columns to retain and sum during duplicate removal. seq\_fields sequence annotation columns to retain and collapse during duplicate removal. Note, this is distinct from the seq and germ arguments, which contain the primary sequence data for the clone and should not be repeated in this argument. if TRUE add an additional annotation column called COLLAPSE\_COUNT during add\_count duplicate removal that indicates the number of sequences that were collapsed. passed on to collapseDuplicates. If TRUE, report the numbers of input, disverbose carded and output sequences; otherwise, process sequences silently. collapse collapse identical sequences? cell name of the column containing cell assignment information locus name of the column containing locus information traits column ids to keep distinct during sequence collapse mod3 pad sequences to length multiple three? randomize randomize sequence order? Important if using PHYLIP use\_regions assign CDR/FWR regions? dup\_singles Duplicate sequences in singleton clones to include them as trees? number of cores to parallelize formatting over. nproc chain if HL, include light chain information if available. heavy name of heavy chain locus (default = "IGH") filterstop only use sequences that do not contain an in-frame stop codon minseq minimum number of sequences per clone split\_light split or lump subgroups? See resolveLightChains. light\_traits Include the traits from the light chain when concatenating and collapsing trees? majoronly only return largest subgroup and sequences without light chains

additional data columns to include in output

columns

getAllSeqs 43

### **Details**

This function is a wrapper for makeAirrClone. Also removes whitespace, ;, :, and = from ids

#### Value

A tibble of airrClone objects containing modified clones.

#### See Also

Executes in order makeAirrClone. Returns a tibble of airrClone objects which serve as input to getTrees and findSwitches.

### **Examples**

```
data(ExampleAirr)
# Select two clones, for demonstration purpose
sel <- c("3170", "3184")
clones <- formatClones(ExampleAirr[ExampleAirr$clone_id %in% sel,],traits="sample_id")</pre>
```

getAllSeqs

Return all tip and internal node sequences

### **Description**

getNodeSeq Sequence retrieval function.

#### **Usage**

```
getAllSeqs(data, imgt_gaps = TRUE)
```

### **Arguments**

data a tibble of airrClone objects with reconstructed trees, the output of getTrees imgt\_gaps include a column of gapped sequences?

### **Details**

Column names: clone\_id = clone id node\_id = name of node, either the sequence name if a tip or Node<number> if internal node node = node number in tree. Tips are nodes 1:<number of tips>. locus = locus of sequence sequence = ungapped sequence, either observed for tips or reconstructed for internal nodes sequence\_alignment = sequence with IMGT gaps (optional)

### Value

A tibble with sequence information for each tip and internal node of a set of trees.

### See Also

```
getTrees getNodeSeq
```

44 getBootstraps

getBootstraps Creates a bootstrap distribution for clone sequence alignments, and returns estimated trees for each bootstrap replicate as a nested list as

a new input tibble column.

## **Description**

getBootstraps Phylogenetic bootstrap function.

## Usage

```
getBootstraps(
  clones,
 bootstraps,
  nproc = 1,
  bootstrap_nodes = TRUE,
  dir = NULL,
  id = NULL,
  build = "pratchet",
  exec = NULL,
  quiet = 0,
  rm_temp = TRUE,
  rep = NULL,
  seq = NULL,
  boot_part = "locus",
 by\_codon = TRUE,
  starting_tree = FALSE,
  switches = FALSE,
)
```

### **Arguments**

clones tibble airrClone objects, the output of formatClones

number of bootstrap replicates to perform
nproc number of cores to parallelize computations

bootstrap\_nodes

a logical if the the nodes for each tree in the trees column (required) should

report their bootstrap value

dir directory where temporary files will be placed (required if igphyml or dnapars

specified)

id unique identifier for this analysis (required if igphyml or dnapars specified)

build program to use for tree building (phangorn, dnapars, igphyml)

exec location of desired phylogenetic executable quiet amount of rubbish to print to console

getDivergence 45

rm_temp	remove temporary files (default=TRUE)
rep	current bootstrap replicate (experimental)
seq	column name containing sequence information
boot_part	is "locus" bootstrap columns for each locus separately
by_codon	a logical if the user wants to bootstrap by codon or by nucleotide. Default (codon based bootstrapping) is TRUE.
starting_tree	An indicator to use the existing trees column as the starting trees for RAxML
switches	a logical indicator to allow findSwitches to do permutations.
	additional arguments to be passed to tree building program

### Value

The input clones tibble with an additional column for the bootstrap replicate trees.

## Description

getDivergence get sum of branch lengths leading from the root of the tree. If the germline sequence is included in the tree, this will equal the germline divergence. If germline removed, this will equal the MRCA divergence

## Usage

```
getDivergence(phy, minlength = 0.001)
```

## **Arguments**

phy Tree object

minlength Branch lengths to collapse in trees

### Value

A named vector of each tip's divergence from the tree's root.

46 getGermline

	getGermline	getGermline get germline segment from specified receptor and segment
--	-------------	--

# Description

getGermline get germline segment from specified receptor and segment

# Usage

```
getGermline(
  receptor,
  references,
  segment,
  field,
  germ_start,
  germ_end,
  germ_length,
  germ_aa_start,
  germ_aa_length,
  amino_acid = FALSE
)
```

# Arguments

receptor	row from AIRR-table containing sequence of interest
references	list of reference segments. Must be specific to locus and segment
segment	Gene segment to search. Must be V, D, or J.
field	Column name for segment gene call (e.g. v_call)
germ_start	Column name of index of segment start within germline segment (e.g. v_germline_start)
germ_end	Similar to germ_start, but specifies end of segment (e.g. v_germline_end)
germ_length	Similar to germ_start, but specifies length of segment (e.g. v_germline_end)
germ_aa_start	Column name of index of segment start within germline segment in AA (if amino_acid=TRUE, e.g. v_germline_start)
germ_aa_length	Similar to germ_start, but specifies length of segment in AA (if amino_acid=TRUE, e.g. v_germline_end)
amino_acid	Perform reconstruction on amino acid sequence (experimental)

# Value

String of germline sequence from specified segment aligned with the sequence in the seq column of receptor.

getNodeSeq 47

getNodeSeq	Return IMGT gapped sequence of specified tree node	

## Description

getNodeSeq Sequence retrieval function.

## Usage

```
getNodeSeq(data, node, tree = NULL, clone = NULL, gaps = TRUE)
```

## Arguments

data	a tibble of airrClone objects, the output of getTrees
node	numeric node in tree (see details)
tree	a phylo tree object containing node
clone	if tree not specified, supply clone ID in data
gaps	add IMGT gaps to output sequences?

## **Details**

Use plotTrees(trees)[[1]] + geom\_label(aes(label=node))+geom\_tippoint() to show node labels, and getNodeSeq to return internal node sequences

## Value

A vector with sequence for each locus at a specified node in tree.

### See Also

getTrees

getPalette	Get a color palette for a predefined set of trait values. defaults to black unless specified.	'Germline'

# Description

getPalette Gets a color palette for a predefined set of trait values

```
getPalette(states, palette)
```

48 getSeq

### **Arguments**

states states in model

palette The colorbrewer palette to use

### Value

A named vector with each state corresponding to a color

## See Also

```
getTrees, plotTrees
```

getSeq

Deprecated! Use getNodeSeq

## Description

getSeq Sequence retrieval function.

## Usage

```
getSeq(data, node, tree = NULL, clone = NULL, gaps = TRUE)
```

## **Arguments**

data a tibble of airrClone objects, the output of getTrees

node numeric node in tree (see details)
tree a phylo tree object containing node

clone if tree not specified, supply clone ID in data

gaps add IMGT gaps to output sequences?

## Value

A vector with sequence for each locus at a specified node in tree.

### See Also

getTrees

getSkylines 49

getSkylines

Make data frames for Bayesian skyline plots

# Description

```
makeSkylines
```

## Usage

```
getSkylines(
   clones,
   dir,
   id,
   time,
   burnin = 10,
   bins = 100,
   verbose = 0,
   forward = TRUE,
   nproc = 1,
   max_height = c("min", "median", "mean", "max")
)
```

## Arguments

clones	clone tibble
dir	directory of BEAST trees file
id	unique identifer for this analysis
time	name of time column
burnin	Burnin percent (default 10)
bins	number of bins for plotting
verbose	if 1, print name of clones
forward	plot in forward or (FALSE) backward time?
nproc	processors for parallelization (by clone)
max_height	max height to use (min, median, mean, max)

## **Details**

Burnin set from readBEAST or getTrees

# Value

Bayesian Skyline values for given clone

50 getSubclones

getSubclones

#' Deprecated! Use resolveLightChains

## Description

getSubClones plots a tree or group of trees

# Usage

```
getSubclones(
  heavy,
  light,
  nproc = 1,
  minseq = 1,
  id = "sequence_id",
  seq = "sequence_alignment",
  clone = "clone_id",
  cell = "cell_id",
  v_call = "v_call",
  j_call = "j_call",
  junc_len = "junction_length",
  nolight = "missing"
)
```

## Arguments

heavy	a tibble containing heavy chain sequences with clone_id
light	a tibble containing light chain sequences
nproc	number of cores for parallelization
minseq	minimum number of sequences per clone
id	name of the column containing sequence identifiers.
seq	name of the column containing observed DNA sequences. All sequences in this column must be multiple aligned.
clone	name of the column containing the identifier for the clone. All entries in this column should be identical.
cell	name of the column containing identifier for cells.
v_call	name of the column containing V-segment allele assignments. All entries in this column should be identical to the gene level.
j_call	name of the column containing J-segment allele assignments. All entries in this column should be identical to the gene level.
junc_len	name of the column containing the length of the junction as a numeric value. All entries in this column should be identical for any given clone.
nolight	string to use to indicate a missing light chain

getSubTaxa 51

## Value

a tibble containing

getSubTaxa

Get the tip labels as part of a clade defined by an internal node

## **Description**

getSubTaxa Gets the tip labels from a clade

## Usage

```
getSubTaxa(node, tree)
```

## **Arguments**

node number that defines the target clade

tree phylo object

#### Value

A vector containing tip labels of the clade

## **Examples**

```
# Get taxa from all subtrees
data(BiopsyTrees)
tree <- BiopsyTrees$trees[[8]]
all_subtrees <- lapply(1:length(tree$nodes), function(x)getSubTaxa(x, tree))</pre>
```

 ${\tt getTimeTrees}$ 

Estimate time trees by running BEAST on each clone Applies XML template to each clone

## Description

getTimeTrees Tree building function.

52 getTimeTrees

### Usage

```
getTimeTrees(
  clones,
  template,
  beast,
  dir,
  id,
  time,
  mcmc_length = 3e+07,
  log_every = "auto",
  burnin = 10,
  trait = NULL,
  resume_clones = NULL,
  nproc = 1,
  quiet = 0,
  rm_temp = FALSE,
  include_germline = TRUE,
  seq = "sequence",
  germline_range = c(-10000, 10000),
  java = TRUE,
  seed = NULL,
  log_target = 10000,
  tree_states = FALSE,
  trees = NULL,
)
```

### **Arguments**

clones a tibble of airrClone objects, the output of formatClones

template XML template

beast location of beast binary directory (beast/bin)
dir directory where temporary files will be placed.

id unique identifer for this analysis
time Name of sample time column
mcmc\_length Number of MCMC steps

log\_every Frequency of states logged. "auto" will divide mcmc\_length by log\_target

burnin Burnin percent (default 10)
trait Trait column to be used

nproc Number of cores for parallelization. At most 1 core/tree can be used.

quiet amount of rubbish to print to console rm\_temp remove temporary files (default=TRUE)

getTimeTreesIterate 53

include\_germline

Include germline sequence in analysis?

seq Sequence column in data

germline\_range Possible date range of germline tip
java Use the -java flag for BEAST run

seed Use specified seeed for the -seed option for BEAST

log\_target Target number of samples from MCMC chain

trees optional list of starting trees, either phylo objects or newick strings

... Additional arguments passed to tree building programs

#### **Details**

For examples and vignettes, see https://dowser.readthedocs.io

## Value

A tibble with a column of phylo objects and parameters column

#### See Also

```
getTrees, readBEAST
```

getTimeTreesIterate

Iteratively resume getTimeTrees until convergence, as defined by all parameters (except those in ignore vector) having ESS greater than or equal to the specified ess\_cutoff

### **Description**

 ${\tt getTimeTreesIterate}\ Iteratively\ resume\ {\tt getTimeTrees}\ til\ convergence.$ 

```
getTimeTreesIterate(
  clones,
  iterations = 10,
  ess_cutoff = 200,
  ignore = c("traitfrequencies"),
  quiet = 0,
  ...
)
```

54 getTrees

## Arguments

clones a tibble of airrClone objects, the output of formatClones iterations Maximum number of times to resume MCMC chain ess\_cutoff Minimum number of ESS for all parameters ignore Vector of parameters to ignore for ESS calculation quiet notifications if > 0... Additional arguments for getTimeTrees

## **Details**

For examples and vignettes, see https://dowser.readthedocs.io

### Value

A tibble of tidytree and airrClone objects.

getTrees

Estimate lineage tree topologies, branch lengths, and internal node states if desired

## **Description**

getTrees Tree building function.

```
getTrees(
  clones,
  trait = NULL,
  id = NULL,
  dir = NULL,
 modelfile = NULL,
  build = "pratchet",
  exec = NULL,
  igphyml = NULL,
  fixtrees = FALSE,
  nproc = 1,
  quiet = 0,
  rm_temp = TRUE,
  palette = NULL,
  seq = NULL,
  collapse = FALSE,
  check_divergence = TRUE,
)
```

getTrees 55

#### **Arguments**

clones a tibble of airrClone objects, the output of formatClones

trait to use for parsimony models (required if igphyml specified)

id unique identifier for this analysis (required if igphyml or dnapars specified)

dir directory where temporary files will be placed.

modelfile file specifying parsimony model to use

build program to use for tree building (pratchet, pml, dnapars, dnaml, igphyml, raxml)

exec location of desired phylogenetic executable

igphyml optional location of igphyml executable for parsimony

fixtrees if TRUE, use supplied tree topologies

nproc number of cores to parallelize computations

quiet amount of rubbish to print to console rm\_temp remove temporary files (default=TRUE)

palette deprecated

seq column name containing sequence information
collapse Collapse internal nodes with identical sequences?

check\_divergence

run checkDivergence on trees?

... Additional arguments passed to tree building programs

#### **Details**

Estimates phylogenetic tree topologies and branch lengths for a list of airrClone objects. By default, it will use phangorn::pratchet to estimate maximum parsimony tree topologies, and ape::acctran to estimate branch lengths. If igpyhml is specified, internal node trait values will be predicted by maximum parsimony. In this case, dir will need to be specified as a temporary directory to place all the intermediate files (will be created if not available). Further, id will need to specified to serve as a unique identifier for the temporary files. This should be chosen to ensure that multiple getTrees calls using the same dir do not overwrite each others files.

modelfile is written automatically if not specified, but doesn't include any constraints. Intermediate files are deleted by default. This can be toggled using (rm\_files).

For examples and vignettes, see https://dowser.readthedocs.io

#### Value

A list of phylo objects in the same order as data.

#### See Also

formatClones, findSwitches, buildPhylo, buildPratchet, buildPML, buildIgphyml, buildRAxML

56 IsotypeTrees

## **Examples**

 ${\tt IsotypeTrees}$ 

Example Ig lineage trees with isotype reconstructions.

## Description

Same as ExampleClones but with isotypes predicted at internal nodes

## Usage

IsotypeTrees

#### **Format**

A tibble of airrClone and phylo objects output by getTrees.

- clone\_id: Clonal cluster
- data: List of airrClone objects
- seqs: Number of sequences
- trees: List of phylo objects

### See Also

IsotypeTrees

makeAirrClone 57

makeAirrClone

Generate a airrClone object for lineage construction

### **Description**

makeAirrClone takes a data.frame with AIRR or Change-O style columns as input and masks gap positions, masks ragged ends, removes duplicates sequences, and merges annotations associated with duplicate sequences. It returns a airrClone object which serves as input for lineage reconstruction.

## Usage

```
makeAirrClone(
  data,
  id = "sequence_id",
  seq = "sequence_alignment",
  germ = "germline_alignment_d_mask",
  v_{call} = "v_{call}",
  j_call = "j_call",
  junc_len = "junction_length",
  clone = "clone_id",
  subgroup = "clone_subgroup",
  mask\_char = "N",
 max_mask = 0,
  pad_end = TRUE,
  text_fields = NULL,
  num_fields = NULL,
  seq_fields = NULL,
  add_count = TRUE,
  verbose = FALSE,
  collapse = TRUE,
  chain = "H",
  heavy = NULL,
  cell = "cell_id",
  locus = "locus",
  traits = NULL,
  mod3 = TRUE,
  randomize = TRUE,
  use_regions = TRUE,
  dup_singles = FALSE,
  light_traits = FALSE
)
```

### **Arguments**

data

data.frame containing the AIRR or Change-O data for a clone. See Details for the list of required columns and their default values.

58 makeAirrClone

id	name of the column containing sequence identifiers.
seq	name of the column containing observed DNA sequences. All sequences in this column must be multiple aligned.
germ	name of the column containing germline DNA sequences. All entries in this column should be identical for any given clone, and they must be multiple aligned with the data in the seq column.
v_call	name of the column containing V-segment allele assignments. All entries in this column should be identical to the gene level.
j_call	name of the column containing J-segment allele assignments. All entries in this column should be identical to the gene level.
junc_len	name of the column containing the length of the junction as a numeric value. All entries in this column should be identical for any given clone.
clone	name of the column containing the identifier for the clone. All entries in this column should be identical.
subgroup	name of the column containing the identifier for the subgroup.
mask_char	character to use for masking and padding.
max_mask	maximum number of characters to mask at the leading and trailing sequence ends. If NULL then the upper masking bound will be automatically determined from the maximum number of observed leading or trailing Ns amongst all sequences. If set to $\theta$ (default) then masking will not be performed.
pad_end	if TRUE pad the end of each sequence with $mask\_char$ to make every sequence the same length.
text_fields	text annotation columns to retain and merge during duplicate removal.
num_fields	numeric annotation columns to retain and sum during duplicate removal.
seq_fields	sequence annotation columns to retain and collapse during duplicate removal. Note, this is distinct from the seq and germ arguments, which contain the primary sequence data for the clone and should not be repeated in this argument.
add_count	if TRUE add an additional annotation column called COLLAPSE_COUNT during duplicate removal that indicates the number of sequences that were collapsed.
verbose	passed on to collapseDuplicates. If TRUE, report the numbers of input, discarded and output sequences; otherwise, process sequences silently.
collapse	collapse identical sequences?
chain	if HL, include light chain information if available.
heavy	name of heavy chain locus (default = "IGH")
cell	name of the column containing cell assignment information
locus	name of the column containing locus information
traits	column ids to keep distinct during sequence collapse
mod3	pad sequences to length multiple three?
randomize	randomize sequence order? Important if using PHYLIP
use_regions	assign CDR/FWR regions?
dup_singles	Duplicate sequences in singleton clones to include them as trees?
light_traits	Include the traits from the light chain when concatenating and collapsing trees?

makeModelFile 59

#### **Details**

The input data.frame (data) must columns for each of the required column name arguments: id, seq, germ, v\_call, j\_call, junc\_len, and clone. Additional annotation columns specified in the traits, text\_fields, num\_fields or seq\_fields arguments will be retained in the data slot of the return object, but are not required. These options differ by their behavior among collapsed sequences. Identical sequences that differ by any values specified in the traits option will be kept distinct. Identical sequences that differ only by values in the num\_fields option will be collapsed and the values of their num\_fields columns will be added together. Similar behavior occurs with text\_fields but the unique values will concatenated with a comma.

The default columns are IMGT-gapped sequence columns, but this is not a requirement. However, all sequences (both observed and germline) must be multiple aligned using some scheme for both proper duplicate removal and lineage reconstruction.

The value for the germline sequence, V-segment gene call, J-segment gene call, junction length, and clone identifier are determined from the first entry in the germ, v\_call, j\_call, junc\_len and clone columns, respectively. For any given clone, each value in these columns should be identical.

To allow for cases where heavy and light chains are used, this function returns three sequence columns for heavy chains (sequence), light chain (lsequence, empty if none available), and concatenated heavy+light chain (hlsequence). These contain sequences in alignment with germline, lgermline, and hlgermline slots, respectively. The sequence column used for build trees is specified in the phylo\_seq slot. Importantly, this column is also the sequence column that also has uninformative columns removed by cleanAlignment. It is highly likely we will change this system to a single sequence and germline slot in the near future.

The airrClone object also contains vectors locus, region, and numbers, which contain the locus, IMGT region, and IMGT number for each position in the sequence column specified in phylo\_seq. If IMGT-gapped sequences are not supplied, this will likely result in an error. Specify use\_regions=FALSE if not using IMGT-gapped sequences

#### Value

A airrClone object containing the modified clone.

#### See Also

Returns an airrClone. See formatClones to generate an ordered list of airrClone objects.

## **Examples**

```
data(ExampleAirr)
airr_clone <- makeAirrClone(ExampleAirr[ExampleAirr$clone_id=="3184",])</pre>
```

makeModelFile

Make a parsimony model file

### **Description**

makeModelFile Filler

60 makeSkyline

### Usage

```
makeModelFile(file, states, constraints = NULL, exceptions = NULL)
```

## **Arguments**

file model file name to write.

states vector of states to include in model.

constraints constraints to add to model.

exceptions vector of comma-separated states that are exceptions to constraints

### **Details**

Currently the only option for constraints is "irrev", which forbids switches moving from left to right in the states vector.

## Value

Name of model file

#### See Also

readModelFile, getTrees, findSwitches

makeSkyline

get values for Bayesian Skyline plot

## **Description**

```
makeSkyline
```

```
makeSkyline(
  logfile,
  treesfile,
  burnin,
  bins = 100,
  youngest = 0,
  clone_id = NULL,
  max_height = c("min", "median", "mean", "max")
)
```

maskCodons 61

## Arguments

logfile Beast log file treesfile BEAST trees file

burnin Burnin percentage (1-100) bins number of bins for plotting

youngest timepoint of the most recently tip sampled (if 0, backward time used)

clone\_id name of the clone being analyzed (if desired)
max\_height max height to use (min, median, mean, max)

### Value

Bayesian Skyline values for given clone

maskCodons

maskCodons Masks codons split by insertions

### **Description**

maskCodons Masks codons split by insertions

### Usage

```
maskCodons(
  id,
  q,
  s,
  keep_alignment = FALSE,
  gap_opening = 5,
  gap_extension = 1,
  keep_insertions = FALSE,
  mask = TRUE
)
```

### **Arguments**

id sequence id

q (query) un-aligned input sequence (sequence)

s (subject) aligned input sequence (sequence\_alignment)

keep\_alignment store q and s alignments

gap\_opening gap opening penalty (Biostrings::pairwiseAlignment)
gap\_extension gap extension penalty (Biostrings::pairwiseAlignment)

keep\_insertions

return removed insertion sequences?

mask if FALSE, don't mask codons

62 maskSequences

### **Details**

Performs global alignment of q and s, masks codons in s that are split by insertions (see example) masking\_note notes codon positions in subject\_alignment sequence that were masked, if found. subject\_alignment contains subject sequence aligned to query (q) sequence query\_alignment contains query sequence aligned to subject (q) sequence sequence\_masked will be NA if frameshift or alignment error detected/

### Value

A list with split codons masked, if found (sequence\_masked).

#### See Also

maskSequences, Biostrings::pairwiseAlignment.

### **Examples**

```
s = "ATCATCATC..."
q = "ATCTTTATCATC"
print(maskCodons(1,q,s,TRUE))

s <- "ATCATCATC..."
q <- "ATTTTCATCATC"
print(maskCodons("test",q,s,keep_alignment=TRUE,keep_insertions=TRUE))</pre>
```

maskSequences

maskSequences Mask codons split by insertions in V gene

#### **Description**

maskSequences Mask codons split by insertions in V gene

```
maskSequences(
  data,
  sequence_id = "sequence_id",
  sequence = "sequence",
  sequence_alignment = "sequence_alignment",
  v_sequence_start = "v_sequence_start",
  v_sequence_end = "v_sequence_end",
  v_germline_start = "v_germline_start",
  v_germline_end = "v_germline_end",
  junction_length = "junction_length",
  keep_alignment = FALSE,
  keep_insertions = FALSE,
  mask_codons = TRUE,
  mask_cdr3 = TRUE,
```

maskSequences 63

```
nproc = 1
)
```

### **Arguments**

data BCR data table sequence id column sequence\_id input sequence column (query) sequence sequence\_alignment aligned (IMGT-gapped) sequence column (subject) v\_sequence\_start V gene start position in sequence v\_sequence\_end V gene end position in sequence v\_germline\_start V gene start position in sequence\_alignment v\_germline\_end V gene end position in sequence alignment junction\_length name of junction\_length column keep\_alignment store alignment of query and subject sequences? keep\_insertions return removed insertion sequences? mask\_codons mask split codons? mask CDR3 sequences? mask\_cdr3

number of cores to use

#### **Details**

nproc

Performs global alignment of sequence and sequence\_alignment, masking codons in sequence\_alignment that are split by insertions (see examples) masking\_note notes codon positions in subject\_alignment sequence that were masked, if found. subject\_alignment contains subject sequence aligned to query sequence (only if keep\_alignment=TRUE) query\_alignment contains query sequence aligned to subject sequence (only if keep\_alignment=TRUE) sequence\_masked will be NA if frameshift or alignment error detected. This will be noted insertions column will be returned if keep\_insertions=TRUE, contains a comma-separated list of each position in query alignment>-<sequence>. See example. in masking note.

## Value

A tibble with masked sequence in sequence\_masked column, as well as other columns.

## See Also

maskCodons, Biostrings::pairwiseAlignment.

plotTrees

plotSkylines

Simple function for plotting Bayesian skyline plots

## Description

```
plotSkylines Simple Bayesian skyline plots
```

### Usage

```
plotSkylines(clones, file = NULL, width = 8.5, height = 11, ...)
```

## **Arguments**

```
clones output from getTrees using BEAST

file pdf file name for printing plots

width width of plot in inches if file specified

height height of plot in inches if file specified

optional arguments passed to grDevices::pdf
```

### Value

if no file specified, a list of ggplot objects. If file specified will plot to specified file

## See Also

getSkylines readBEAST getTrees

plotTrees

Plot a tree with colored internal node labels using ggtree

## **Description**

plotTrees plots a tree or group of trees

```
plotTrees(
   trees,
   nodes = FALSE,
   tips = NULL,
   tipsize = NULL,
   scale = 0.01,
   palette = "Dark2",
   base = FALSE,
   layout = "rectangular",
```

plotTrees 65

```
node_nums = FALSE,
tip_nums = FALSE,
title = TRUE,
labelsize = NULL,
common_scale = FALSE,
ambig = "grey",
bootstrap_scores = FALSE,
tip_palette = NULL,
node_palette = NULL,
guide_title = NULL,
branch_lengths = NULL)
```

### **Arguments**

trees A tibble containing phylo and airrClone objects

nodes color internal nodes if possible?

tips color tips if possible? tipsize size of tip shape objects

scale width of branch length scale bar

palette color palette for tips and/or nodes. Can supply a named vector for all tip states,

or a palette named passed to ggplot2::scale\_color\_brewer (e.g. "Dark2", "Paired",

"Set1") or ggplot2::scale\_color\_distiller (e.g. RdYlBu) or

base recursion base case (don't edit)
layout rectangular or circular tree layout?

node\_nums plot internal node numbers?

tip\_nums plot tip numbers? title use clone id as title?

labelsize text size

common\_scale stretch plots so branches are on same scale? determined by sequence with high-

est divergence

ambig How to color ambiguous node reconstructions? (grey or blend)

bootstrap\_scores

Show bootstrap scores for internal nodes? See getBootstraps.

tip\_palette deprecated, use palette node\_palette deprecated, use palette

guide\_title Title of color guide. Defaults to tips variable if specified.

branch\_lengths Use branch lenghts? Use "none" if not.

#### **Details**

Function uses ggtree functions to plot tree topologies estimated by getTrees, and findSwitches. Object can be further modified with ggtree functions. Please check out https://bioconductor.org/packages/devel/bioc/vignettes/g and cite ggtree in addition to dowser if you use this function.

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## Value

a grob containing a tree plotted by ggtree.

#### See Also

```
getTrees, findSwitches
```

## **Examples**

```
data(ExampleClones)
trees <- getTrees(ExampleClones[10,])
plotTrees(trees)[[1]]</pre>
```

readBEAST

Reads in a BEAST output directory

## **Description**

readBEAST Reads in data from BEAST output directory

### Usage

```
readBEAST(
  clones,
  dir,
  id,
  beast,
  burnin = 10,
  trait = NULL,
  nproc = 1,
  quiet = 0,
  full_posterior = FALSE,
  asr = FALSE,
  low_ram = TRUE
)
```

## **Arguments**

clones	either a tibble (getTrees) or list of airrClone objects
dir	directory where BEAST output files have been placed.
id	unique identifer for this analysis

unique identifier for this analysis

beast location of beast binary directory (beast/bin)

burnin percent of initial tree samples to discard (default 10)

trait Trait coolumn used

nproc Number of cores for parallelization. Uses at most 1 core per tree.

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quiet amount of rubbish to print to console

full\_posterior Read un full distribution of parameters and trees?

asr Log ancestral sequences?

low\_ram run with less memory (slightly slower)

#### Value

If data is a tibble, then the input clones tibble with additional columns for trees and parameter estimates given the specified burnin. If input is just a list of airrClone objects, it will return the corresponding list of trees given the burnin

readFasta

Read a fasta file into a list of sequences readFasta reads a fasta file

### **Description**

Read a fasta file into a list of sequences readFasta reads a fasta file

### Usage

```
readFasta(file)
```

## **Arguments**

file FASTA file

#### Value

List of sequences

readIMGT

readIMGT read in IMGT database

## Description

Loads all reference germlines from an Immcantation-formatted IMGT database.

## Usage

```
readIMGT(dir, quiet = FALSE)
```

## Arguments

dir directory containing Immcantation-formatted IMGT database

quiet print warnings?

68 readLineages

### **Details**

Input directory must be formatted to Immcantation standard. See https://changeo.readthedocs.io/en/stable/examples/igblast.h for example of how to download.

#### Value

List of lists, leading to IMGT-gapped nucleotide sequences. Structure of object is list[[locus]][[segment]] locus refers to locus (e.g. IGH, IGK, TRA) segment refers to gene segment category (V, D, or J)

## **Examples**

```
# vdj_dir contains a minimal example of reference germlines
# (IGHV3-11*05, IGHD3-10*01 and IGHJ5*02)
# which are the gene assignments for ExampleDb[1,]
vdj_dir <- system.file("extdata", "germlines", "imgt", "human", "vdj", package="dowser")
imgt <- readIMGT(vdj_dir)</pre>
```

readLineages

Read in all trees from a lineages file

### **Description**

Read in all trees from a lineages file

### Usage

```
readLineages(
   file,
   states = NULL,
   palette = NULL,
   run_id = "",
   quiet = TRUE,
   append = NULL,
   format = "nexus",
   type = "jointpars")
```

#### **Arguments**

```
file
                  IgPhyML lineage file
states
                  states in parsimony model
palette
                  deprecated
run_id
                  id used for IgPhyML run
                  avoid printing rubbish on screen?
quiet
append
                  string appended to fasta files
format
                  format of input file with trees
type
                  Read in parsimony reconstructions or ancestral sequence reconstructions? "joint-
                  pars" reads in parsimony states, others read in sequences in internal nodes
```

readModelFile 69

## Value

A list of phylo objects from file.

readModelFile

Read in a parsimony model file

## Description

```
readModelFile Filler
```

## Usage

```
readModelFile(file, useambig = FALSE)
```

## **Arguments**

file parsimony model file.

use ambiguous naming as specified in the file?

### Value

A named vector containing the states of the model

#### See Also

make Model File, find Switches, get Trees

reconIgPhyML

Do IgPhyML maximum parsimony reconstruction

## Description

reconIgPhyML IgPhyML parsimony reconstruction function

```
reconIgPhyML(
  file,
  modelfile,
  id,
  igphyml = "igphyml",
  mode = "switches",
  type = "recon",
  nproc = 1,
  quiet = 0,
```

70 rerootTree

```
rm_files = FALSE,
  rm_dir = NULL,
  states = NULL,
  palette = NULL,
  resolve = 2,
  rseed = NULL,
  force_resolve = FALSE,
)
```

## **Arguments**

file IgPhyML lineage file (see writeLineageFile)

modelfile File specifying parsimony model

id for IgPhyML run id

location of igphyml executable igphyml

return trees or count switches? (switches or trees) mode

get observed switches or permuted switches? type

cores to use for parallelization nproc amount of rubbish to print quiet rm\_files remove temporary files? remove temporary directory? rm\_dir

states in parsimony model states

palette deprecated

resolve level of polytomy resolution. 0=none, 1=maximum parsimony, 2=maximum

ambiguity

rseed random number seed if desired

force\_resolve continue even if polytomy resolution fails?

additional arguments

### Value

Either a tibble of switch counts or a list of trees with internal nodes predicted by parsimony.

rerootTree	Reroot phyloge	enetic tree to	have its germline	sequence at a zero-length	ı

branch to a node which is the direct ancestor of the tree's UCA. Assigns uca to be the ancestral node to the tree's germline sequence, as

germid as the tree's germline sequence ID.

resolveLightChains 71

### **Description**

Reroot phylogenetic tree to have its germline sequence at a zero-length branch to a node which is the direct ancestor of the tree's UCA. Assigns uca to be the ancestral node to the tree's germline sequence, as germid as the tree's germline sequence ID.

## Usage

```
rerootTree(tree, germline, min = 0.001, verbose = 1)
```

### **Arguments**

tree An ape phylo object

germline ID of the tree's predicted germline sequence

min Maximum allowed branch length from germline to root

verbose amount of rubbish to print

### Value

phylo object rooted at the specified germline

 ${\tt resolveLightChains}$ 

Define subgroups within clones based on light chain rearrangements

# Description

resolveLightChains resolve light chain V and J subgroups within a clone

```
resolveLightChains(
  data,
  nproc = 1,
 minseq = 1,
 locus = "locus",
  heavy = "IGH",
  id = "sequence_id",
  seq = "sequence_alignment",
  clone = "clone_id",
  cell = "cell_id",
  v_call = "v_call"
  j_call = "j_call",
  junc_len = "junction_length",
 nolight = "missing",
  pad_ends = TRUE
)
```

72 resolveLightChains

### **Arguments**

data	a tibble containing heavy and light chain sequences with clone_id
nproc	number of cores for parallelization
minseq	minimum number of sequences per clone
locus	name of column containing locus values
heavy	value of heavy chains in locus column. All other values will be treated as light chains
id	name of the column containing sequence identifiers.
seq	name of the column containing observed DNA sequences. All sequences in this column must be multiple aligned.
clone	name of the column containing the identifier for the clone. All entries in this column should be identical.
cell	name of the column containing identifier for cells.
v_call	name of the column containing V-segment allele assignments. All entries in this column should be identical to the gene level.
j_call	name of the column containing J-segment allele assignments. All entries in this column should be identical to the gene level.
junc_len	name of the column containing the length of the junction as a numeric value. All entries in this column should be identical for any given clone.
nolight	string to use to indicate a missing light chain
pad_ends	pad sequences within a clone to same length?

### **Details**

1. Make temporary array containing light chain clones 2. Enumerate all possible V, J, and junction length combinations 3. Determine which combination is the most frequent 4. Assign sequences with that combination to clone t 5. Copy those sequences to return array 6. Remove all cells with that combination from temp array 7. Repeat 1-6 until temporary array zero. If there is more than rearrangement with the same V/J in the same cell, pick the one with the highest non-ambiguous characters. Cells with missing light chains are grouped with their subgroup with the closest matching heavy chain (Hamming distance) then the largest and lowest index subgroup if ties are present.

Outputs of the function are 1. clone\_subgroup which identifies the light chain VJ rearrangement that sequence belongs to within it's clone 2. clone\_subgroup\_id which combines the clone\_id variable and the clone\_subgroup variable by a "\_". 3. vj\_cell which combines the vj\_gene and vj\_alt\_cell columns by a ",".

#### Value

a tibble containing the same data as inputting, but with the column clone\_subgroup added. This column contains subgroups within clones that contain distinct light chain V and J genes, with at most one light chain per cell.

resolvePolytomies 73

resolvePolytomies Resolve polytomies to have the minimum number of single timepoint clades	resolvePolytomies	, , , , , , , , , , , , , , , , , , ,
--	-------------------	---------------------------------------

## Description

Resolve polytomies to have the minimum number of single timepoint clades

## Usage

```
resolvePolytomies(
  phy,
  clone,
  minlength = 0.001,
  time = "time",
  sequence = "sequence_id",
  germline = "Germline",
  verbose = FALSE
)
```

## **Arguments**

phy	Tree object	
clone	airrClone data object corresponding to phy	
minlength	Branch lengths to collapse in trees	
time	Column name holding numeric time information	
sequence	Column name holding sequence ID	
germline	Germline sequence name	
verbose	Print lots of rubbish while running?	

## **Details**

Iteratively identifies polytomies (clusters of < minlength branches), prunes each descendant branch, combines clades with the same timepoint before grouping them back together. Checks to make sure that the divergence of each tip is the same after resolution.

## Value

A phylo tree object in which polytomies are resolved to have the minimum number of single time-point clades.

## See Also

Uses output from getTrees during correlationTest.

74 runCorrelationTest

## **Description**

runCorrelationTest performs root-to-tip regression permutation test

## Usage

```
runCorrelationTest(
  phy,
  clone,
  permutations,
  minlength = 0.001,
  polyresolve = TRUE,
  permutation = c("clustered", "uniform"),
  time = "time",
  sequence = "sequence_id",
  germline = "Germline",
  verbose = TRUE,
  alternative = c("greater", "two.sided")
)
```

## **Arguments**

phy Tree object

clone airrClone data object corresponding to phy

permutations Number of permutations to run
minlength Branch lengths to collapse in trees

polyresolve Resolve polytomies to have a minimum number of single timepoint clades

permutation Permute among single timepoint clades or uniformly among tips

time Column name holding numeric time information

sequence Column name holding sequence ID

germline Germline sequence name

verbose Print lots of rubbish while running?

alternative Is alternative that the randomized correlation are greater than or equal to ob-

served, or greater/less than?

#### **Details**

See correlationTest for details

## Value

A list of statistics from running the permutation test.

#### See Also

correlationTest.

sampleCloneMultiGroup SampleCloneMultiGroup Down-sample clone to specified size with one or multiple groups to sample evenly

## Description

sampleCloneMultiGroup Down-sample clone to specified size with one or multiple groups to sample evenly

#### Usage

```
sampleCloneMultiGroup(clone, size, weight = NULL, group = NULL)
```

## **Arguments**

clone an airrClone object

size target size

weight column for weighting sample probability group column(s) to sample evenly among group

## Value

a down-sampled airrClone object

sampleClones

sampleClones Down-sample clones to specified size

## **Description**

sampleClones Down-sample clones to specified size

## Usage

```
sampleClones(clones, size, weight = NULL, group = NULL)
```

76 scaleBranches

#### **Arguments**

clones a tibble of airrClone objects

size target size

weight column for weighting sample probability

group column (or columns) to sample evenly among groups

#### Value

The input object with sequences down-sampled

scaleBranches Scale branch lengths to represent either mutations or mutations per

site.

# Description

scaleBranches Branch length scaling function.

## Usage

```
scaleBranches(clones, edge_type = "mutations")
```

## Arguments

clones a tibble of airrClone and phylo objects, the output of getTrees.

edge\_type Either genetic\_distance (mutations per site) or mutations

## **Details**

Uses clones\$trees[[1]]\$edge\_type to determine how branches are currently scaled.

## Value

A tibble with phylo objects that have had branch lengths rescaled as specified.

#### See Also

getTrees

stitchRegions 77

stitchRegions	stitchRegions Similar to stitchVDJ but with segment IDs instead of nucleotides

## Description

stitchRegions Similar to stitchVDJ but with segment IDs instead of nucleotides

# Usage

```
stitchRegions(
  receptor,
  v_seq,
 d_seq,
  j_seq,
  np1_length = "np1_length",
  np2_length = "np1_length",
  n1_length = "n1_length",
 p3v_length = "p3v_length",
 p5d_length = "p5d_length",
 p3d_length = "p3d_length",
  n2_length = "n2_length",
  p5j_length = "p5j_length",
  np1_aa_length = "np1_aa_length",
  np2_aa_length = "np2_aa_length",
  amino_acid = FALSE
)
```

receptor	row from AIRR-table containing sequence of interest
Гесерсог	
v_seq	germline V segment sequence from getGermline
d_seq	germline D segment sequence from getGermline
j_seq	germline J segment sequence from getGermline
np1_length	Column name in receptor specifying np1 segment length (e.g. np1_length)
np2_length	Column name in receptor specifying np2 segment length (e.g. np1_length)
n1_length	Column name in receptor specifying n1 segment length (experimental)
p3v_length	Column name in receptor specifying p3v segment length (experimental)
p5d_length	Column name in receptor specifying p5d segment length (experimental)
p3d_length	Column name in receptor specifying p3d segment length (experimental)
n2_length	Column name in receptor specifying n2 segment length (experimental)
p5j_length	Column name in receptor specifying p5j segment length (experimental)
np1_aa_length	Column name in receptor specifying np1 segment length in AA (if amino_acid=TRUE, e.g. np1_length)

78 stitchVDJ

```
np2_aa_length Column name in receptor specifying np2 segment length in AA (if amino_acid=TRUE, e.g. np1_length)

amino_acid Perform reconstruction on amino acid sequence (experimental)
```

#### Value

Full length germline VDJ sequence with segment IDs instead of nucleotides.

#### See Also

stitchVDJ

stitchVDJ

stitchVDJ combines germline gene segments to a single string

## Description

stitchVDJ combines germline gene segments to a single string

#### Usage

```
stitchVDJ(
  receptor,
  v_seq,
  d_seq,
  j_seq,
  np1_length = "np1_length",
  np2_length = "np2_length",
  np1_aa_length = "np1_aa_length",
  np2_aa_length = "np2_aa_length",
  amino_acid = FALSE
)
```

```
receptor
                 row from AIRR-table containing sequence of interest
v_seq
                 germline V segment sequence from getGermline
d_seq
                 germline D segment sequence from getGermline
                 germline J segment sequence from getGermline
j_seq
np1_length
                  Column name in receptor specifying np1 segment length (e.g. np1_length)
np2_length
                 Column name in receptor specifying np2 segment length (e.g. np1_length)
np1_aa_length
                 Column name in receptor specifying np1 segment length in AA (if amino_acid=TRUE,
                 e.g. np1_length)
                 Column name in receptor specifying np2 segment length in AA (if amino_acid=TRUE,
np2_aa_length
                 e.g. np1 length)
amino_acid
                 Perform reconstruction on amino acid sequence (experimental)
```

stopCodonCheck 79

## Value

Full length germline VDJ sequence aligned with aligned with the sequence in the seq column of receptor.

stopCodonCheck Check whether sequences have in-frame premature stop codons (PTCs)

## Description

Check whether sequences have in-frame premature stop codons (PTCs)

## Usage

```
stopCodonCheck(sequences, nproc = 1, check = TRUE)
```

## Arguments

sequences Vector of nucleotide sequences in desired reading frame

nproc Number of cores for preprocessing check Check whether codons split correctly

## Value

Boolean vector of whether each sequence has an in-frame PTC

testPS

Performs PS (parsimony score) test on switch data

## Description

```
testPS performs a PS test
```

## Usage

```
testPS(
   switches,
   bylineage = FALSE,
   pseudocount = 0,
   alternative = c("less", "two.sided", "greater")
)
```

80 testPS

## **Arguments**

switches Data frame from findSwitches

bylineage Perform test for each lineage individually? (FALSE)

pseudocount Pseudocount for P value calculations

alternative Perform one-sided (greater or less) or two. sided test

#### **Details**

Output data table columns: RECON = PS for observed data PERMUTE = PS for permuted data DELTA = RECON - PERMUTE PLT = p value for DELTA < 0 PGT = p value for DELTA < 0

• RECON: PS for observed data.

• PERMUTE: PS for permuted data.

• DELTA: RECON - PERMUTE.

• PLT: p value that DELTA < 0

• PGT: p value that DELTA > 0

• STAT: Statistic used (PS).

• REP: Bootstrap repetition.

• REPS: Total number of bootstrap repetition.

#### Value

A list containing a tibble with mean PS statistics, and another with PS statistics per repetition.

#### See Also

Uses output from findSwitches. Related to testSP and testSC.

#### **Examples**

```
## Not run:
igphyml <- "~/apps/igphyml/src/igphyml"
data(ExampleAirr)
ExampleAirr$sample_id <- sample(ExampleAirr$sample_id)
clones <- formatClones(ExampleAirr, trait="sample_id")
btrees <- findSwitches(clones[1:2], bootstraps=10, nproc=1,
    igphyml=igphyml, trait="sample_id")
testPS(btrees$switches)
## End(Not run)</pre>
```

testSC 81

testSC

Performs SC (switch count) test on switch data

#### **Description**

```
testSC performs an SC test
```

#### Usage

```
testSC(
   switches,
   dropzeroes = TRUE,
   bylineage = FALSE,
   pseudocount = 0,
   from = NULL,
   to = NULL,
   permuteAll = FALSE,
   alternative = c("two.sided", "greater", "less")
```

## **Arguments**

switches Data frame from findSwitches dropzeroes Drop switches with zero counts?

bylineage Perform test for each lineage individually?
pseudocount Pseudocount for P value calculations
from Include only switches from this state?
to Include only switches to this state?

permuteAll Permute among trees?

alternative Perform one-sided (greater or less) or two.sided test

#### **Details**

Output data table columns: RECON = SC for observed data PERMUTE = SC for permuted data DELTA = RECON - PERMUTE PLT = p value for DELTA < 0 PGT = p value for DELTA < 0

- FROM: State going from.
- T0: State going to.
- RECON: SC for observed data.
- PERMUTE: SC for permuted data.
- DELTA: RECON PERMUTE.
- PLT: p value that DELTA < 0
- PGT: p value that DELTA > 0
- STAT: Statistic used (SC).
- REP: Bootstrap repetition.
- REPS: Total number of bootstrap repetition.

82 testSP

#### Value

A list containing a tibble with mean SC statistics, and another with SC statistics per repetition.

#### See Also

Uses output from findSwitches. Related to testPS and testSP.

#### **Examples**

```
## Not run:
igphyml <- "~/apps/igphyml/src/igphyml"
data(ExampleAirr)
ExampleAirr$sample_id = sample(ExampleAirr$sample_id)
clones = formatClones(ExampleAirr, trait="sample_id")
btrees = findSwitches(clones[1:2], bootstraps=100, nproc=1,
    igphyml=igphyml, trait="sample_id", id="temp", dir="temp")
testSC(btrees$switches)
## End(Not run)</pre>
```

testSP

Performs SP (switch proportion) test on switch data

## **Description**

testSP performs an SP test

#### Usage

```
testSP(
   switches,
   permuteAll = FALSE,
   from = NULL,
   to = NULL,
   dropzeroes = TRUE,
   bylineage = FALSE,
   pseudocount = 0,
   alternative = c("greater", "two.sided", "less"),
   tip_switch = 20,
   exclude = FALSE
)
```

# Arguments

switches Data frame from findSwitches permuteAll Permute among trees?

from Include only switches from this state?

testSP 83

to Include only switches to this state?

dropzeroes Drop switches with zero counts?

bylineage Perform test for each lineage individually?

pseudocount Pseudocount for P value calculations

alternative Perform one-sided (greater or less) or two.sided test

tip\_switch maximum tip/switch ratio

exclude exclude clones with tip/switch ratio > tip\_switch?

#### **Details**

Output data table columns: RECON = SP for observed data PERMUTE = SP for permuted data DELTA = RECON - PERMUTE PLT = p value for DELTA < 0 PGT = p value for DELTA < 0

• FROM: State going from.

• T0: State going to.

• RECON: SP for observed data.

• PERMUTE: SP for permuted data.

• DELTA: RECON - PERMUTE.

• PLT: p value that DELTA < 0

• PGT: p value that DELTA > 0

• STAT: Statistic used (SP).

• REP: Bootstrap repetition.

• REPS: Total number of bootstrap repetition.

## Value

A list containing a tibble with mean SP statistics, and another with SP statistics per repetition.

## See Also

Uses output from findSwitches. Related to testPS and testSC.

## **Examples**

```
## Not run:
igphyml <- "~/apps/igphyml/src/igphyml"
data(ExampleAirr)
ExampleAirr$sample_id = sample(ExampleAirr$sample_id)
clones = formatClones(ExampleAirr, trait="sample_id")
btrees = findSwitches(clones[1:2], bootstraps=10, nproc=1,
    igphyml=igphyml, trait="sample_id")
testSP(btrees$switches)
## End(Not run)</pre>
```

84 treesToPDF

TimeTrees

Example Ig lineage trees sampled over time.

## Description

Same as ExampleClones but with timepoint as a trait value

## Usage

TimeTrees

#### **Format**

A tibble of airrClone and phylo objects output by getTrees.

• clone\_id: Clonal cluster

• data: List of airrClone objects

• seqs: Number of sequences

• trees: List of phylo objects

#### See Also

**TimeTrees** 

treesToPDF

Simple function for plotting a lot of trees into a pdf

## **Description**

treesToPDF exports trees to a pdf in an orderly fashion

## Usage

```
treesToPDF(plots, file, nrow = 2, ncol = 2, ...)
```

# Arguments

plots	list of tree plots (from plotTrees)
file	output file name
nrow	number of rows per page
ncol	number of columns per page

... optional arguments passed to grDevices::pdf

writeCloneSequences 85

## Value

```
a PDF of tree plots
```

## See Also

plotTrees

## **Examples**

```
## Not run:
data(ExampleClones)
trees <- getTrees(ExampleClones[10,])
plots <- plotTrees(trees)
treesToPDF(plots,"test.pdf",width=5,height=6)
## End(Not run)</pre>
```

writeCloneSequences

Write the sequences used in tree building to a fasta format. If there are more than one tree in airrClone output the sequence id will be followed by "\clone\_id".

## Description

writeCloneSequences Exports the sequences used in tree building.

## Usage

```
writeCloneSequences(clones, file)
```

## **Arguments**

 ${\tt clones} \qquad \qquad {\tt tibble\ airrClone\ objects,\ the\ output\ of\ formatClones}$ 

file The file path and name of where the sequences will be saved

writeLineageFile Write lineage file for IgPhyML use

## Description

Write lineage file for IgPhyML use

86 write\_clones\_to\_xmls

## Usage

```
writeLineageFile(
  data,
  trees = NULL,
  dir = ".",
  id = "N",
  rep = NULL,
  trait = NULL,
  empty = TRUE,
  partition = "single",
  heavy = "IGH",
  ...
)
```

# Arguments

data	list of airrClone objects	
trees	list of phylo objects corresponding to data	
dir	directory to write file	
id	id used for IgPhyML run	
rep	bootstrap replicate	
trait	string appended to sequence id in fasta files	
empty	output uninformative sequences?	
partition	how to partition omegas	
heavy	name of heavy chain locus	
	additional arguments to be passed	

## Value

Name of created lineage file.

 $write\_clones\_to\_xmls \quad \textit{Wrapper to write multiple clones to XML files}$ 

# Description

Wrapper to write multiple clones to XML files

write\_clones\_to\_xmls 87

#### Usage

```
write_clones_to_xmls(
  data,
  id,
  trees = NULL,
  time = NULL,
  trait = NULL,
  template = NULL,
  outfile = NULL,
  replacements = NULL,
  trait_list = NULL,
  mcmc_length = 1e+06,
  log_{every} = 1000,
  include_germline_as_root = FALSE,
  include_germline_as_tip = FALSE,
  germline_range = c(-10000, 10000),
  tree_states = FALSE,
  start_edge_length = 100,
  start_date = NULL,
 max_start_date = NULL,
)
```

```
data
                  a list of airrClone objects
                  identifer for this analysis
id
                  optional list of starting trees, either phylo objects or newick strings
trees
                  name of column representing sample time
time
                  name of column representing a trait
trait
template
                  XML template
outfile
                  output file path prefix
replacements
                  list of additional replacements to make in the template
trait_list
                  list of all possible trait values
mcmc_length
                  number of MCMC iterations
log_every
                  frequency of states logged. auto will divide mcmc_length by log_target
include_germline_as_root
                  include germline in analysis as root?
include_germline_as_tip
                  include germline in analysis as tip?
germline_range possible date range of germline
tree_states
                  use states in the starting tree?
start_edge_length
                  edge length to use for all branches in starting tree
```

88 write\_clone\_to\_xml

```
start_date starting date to use as prior, in forward time
max_start_date max starting date to use as prior, in forward time
... additional arguments for XML writing functions
```

## Value

File paths of the written XML files

## **Description**

Takes an airr clone object and template and writes a BEAST2 XML file

## Usage

```
write_clone_to_xml(
  clone,
  file,
  id,
  time = NULL,
  trait = NULL,
  trait_data_type = NULL,
  template = NULL,
 mcmc_length = 1e+06,
 log_{every} = 1000,
  replacements = NULL,
  include_germline_as_root = FALSE,
  include_germline_as_tip = FALSE,
  germline_range = c(-10000, 10000),
  tree = NULL,
  trait_list = NULL,
  log_every_trait = 10,
  tree_states = FALSE,
  start_edge_length = 100,
  start_date = NULL,
 max_start_date = NULL,
)
```

```
clone an airrClone object file output file path
```

write\_clone\_to\_xml 89

id unique identifer for this analysis

time name of column representing sample time

trait name of column representing a trait

trait\_data\_type

optional data type for the trait

template XML template

mcmc\_length number of MCMC iterations

log\_every frequency of states logged. auto will divide mcmc\_length by log\_target

replacements list of additional replacements to make in the template

include\_germline\_as\_root

include germline in analysis as root?

include\_germline\_as\_tip

include germline in analysis as tip?

germline\_range possible date range of germline

tree starting tree, either a phylo object or a newick string

trait\_list list of all possible trait values

log\_every\_trait

frequency of trait states logged relative to log\_every

tree\_states use states in the starting tree?

start\_edge\_length

edge length to use for all branches in starting tree

start\_date starting date to use as prior, in forward time
max\_start\_date max starting date to use as prior, in forward time
... additional arguments for XML writing functions

#### Value

File path of the written XML file

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