TCREMP and TCRpMHC structures

M.S.

2025-01-18

Fetch list of TCRs and their structures from VDJdb

```r
download.file('https://raw.githubusercontent.com/antigenomics/vdjdb-db/refs/heads/master/chunks/PDB_Data
              destfile = "v_tcrpmhc_raw.txt",
              method = "wget")

vpdb <- read_tsv("v_tcrpmhc_raw.txt") |>
  mutate(meta.structure.id = ifelse(meta.structure.id == '4E+41',
                                    "4e41",
                                    meta.structure.id))
```

```
## New names:
## Rows: 284 Columns: 33
## -- Column specification
## -------------------------------------------------------- Delimiter: "\t" chr
## (23): cdr3.alpha, v.alpha, j.alpha, cdr3.beta, v.beta, d.beta, j.beta, s... dbl
## (1): ...1 lgl (9): method.frequency, meta.study.id, meta.cell.subset,
## meta.subset.fre...
## i Use `spec()` to retrieve the full column specification for this data. i
## Specify the column types or set `show_col_types = FALSE` to quiet this message.
## * `` -> `...1`
```

```r
vpdb_meta <- vpdb |>
  select(mhc.class, clone_id = meta.structure.id) |>
  unique()

glimpse(vpdb)
```

```
## Rows: 284
## Columns: 33
## $ ...1               <dbl> 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14~
## $ cdr3.alpha         <chr> "CAVTTDSWGKLQF", "CAAMEGAQKLVF", "CAATGSFNKLTF",~
## $ v.alpha            <chr> "TRAV12-2*01", "TRAV29DV5*01", "TRAV14D-2*01", "~
## $ j.alpha            <chr> "TRAJ24*01", "TRAJ54*01", "TRAJ4*01", "TRAJ32*01~
## $ cdr3.beta          <chr> "CASRPGLAGGRPEQYF", "CASSYPGGGFYEQYF", "CASGGQGR~
## $ v.beta             <chr> "TRBV6-5*01", "TRBV6-5*01", "TRBV13-2*01", "TRBV~
## $ d.beta             <chr> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ j.beta             <chr> "TRBJ2-7*01", "TRBJ2-7*01", "TRBJ2-1*01", "TRBJ1~
## $ species            <chr> "HomoSapiens", "HomoSapiens", "MusMusculus", "Mu~
## $ mhc.a              <chr> "HLA-A*02:01:59", "HLA-A*02:01:48", "H-2Aa", "H-~
## $ mhc.b              <chr> "B2M", "B2M", "H-2Aa", "B2M", "HLA-DRB1*01:01:01~
```

```
## $ mhc.class            <chr> "MHCI", "MHCI", "MHCII", "MHCI", "MHCII", "MHCI"~
## $ antigen.epitope      <chr> "LLFGYPVYV", "LLFGYPVYV", "GNSHRGAIEWEGIESG", "I~
## $ antigen.gene         <chr> "Tax", "Tax", "Ovotransferrin", "Kctd20", "HA", ~
## $ antigen.species      <chr> "HTLV-1", "HTLV-1", "GallusGallus", "MusMusculus~
## $ reference.id         <chr> "PMID:8906788", "PMID:9586631", "PMID:10583947",~
## $ method.identification <chr> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ method.frequency     <lgl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ method.singlecell    <chr> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ method.sequencing    <chr> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ method.verification  <chr> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ meta.study.id        <lgl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ meta.cell.subset     <lgl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ meta.subset.frequency <lgl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ meta.subject.cohort  <chr> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ meta.subject.id      <lgl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ meta.replica.id      <lgl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ meta.clone.id        <chr> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ meta.epitope.id      <lgl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ meta.tissue          <chr> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ meta.donor.MHC       <lgl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ meta.donor.MHC.method <lgl> NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, NA, ~
## $ meta.structure.id    <chr> "1ao7", "1bd2", "1d9k", "1fo0", "1fyt", "1g6r", ~
```

Format into AIRR

```
vpdb <- vpdb |>
  filter(species == "HomoSapiens") |>
  pivot_longer(cols = c(v.alpha, j.alpha, cdr3.alpha,
                        v.beta, j.beta, cdr3.beta)) |>
  select(meta.structure.id, name, value) |>
  separate(name, c("variable", "locus")) |>
  unique() |>
  pivot_wider(id_cols = c(meta.structure.id, locus),
              names_from = variable,
              values_from = value) |>
  rename(clone_id = meta.structure.id,
         v_call = v, j_call = j,
         junction_aa = cdr3)

write_tsv(vpdb, "v_tcrpmhc.txt")
glimpse(vpdb)
```

```
## Rows: 432
## Columns: 5
## $ clone_id    <chr> "1ao7", "1ao7", "1bd2", "1bd2", "1fyt", "1fyt", "1j8h", "1~
## $ locus       <chr> "alpha", "beta", "alpha", "beta", "alpha", "beta", "alpha"~
## $ v_call      <chr> "TRAV12-2*01", "TRBV6-5*01", "TRAV29DV5*01", "TRBV6-5*01",~
## $ j_call      <chr> "TRAJ24*01", "TRBJ2-7*01", "TRAJ54*01", "TRBJ2-7*01", "TRA~
## $ junction_aa <chr> "CAVTTDSWGKLQF", "CASRPGLAGGRPEQYF", "CAAMEGAQKLVF", "CASS~
```

Download PDB structures

```r
pdb_ids <- unique(vpdb$clone_id)
pdb_files <- get.pdb(pdb_ids, path = "tmp/")
```

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1ao7.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1bd2.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1fyt.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1j8h.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1mi5.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1oga.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1qrn.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1qse.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1qsf.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1zgl.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2ak4.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2bnq.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2bnr.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2esv.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2f53.pdb exists. Skipping
download

Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2f54.pdb exists. Skipping
download

```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2gj6.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2iam.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2ian.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2nx5.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2p5e.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2p5w.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2pye.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2vlj.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2vlk.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2vlr.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2xn9.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2ypl.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3d39.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3d3v.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3dxa.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3ffc.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3gsn.pdb exists. Skipping
## download
```

```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3h9s.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3hg1.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3kpr.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3kps.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3kxf.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3mv7.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3mv8.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3mv9.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3o4l.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3pwp.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3qdg.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3qdj.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3qdm.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3qeq.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3qfj.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3sjv.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3uts.pdb exists. Skipping
## download
```

```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3utt.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3vxm.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3vxr.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3vxs.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4c56.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4e41.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4eup.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4ftv.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4g8g.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4g9f.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4gg6.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4jfd.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4jfe.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4jff.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4jrx.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4jry.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4l3e.pdb exists. Skipping
## download
```

```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4mji.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4mnq.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4ozf.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4ozg.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4ozh.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4ozi.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4prh.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4pri.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4prp.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4qok.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4qrp.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4y19.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4y1a.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4z7u.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4z7v.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4z7w.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5d2l.pdb exists. Skipping
## download
```

```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5d2n.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1lp9.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1ymm.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2j8u.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2jcc.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2uwe.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2wbj.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3gjf.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3hae.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3nfj.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3o6f.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3pl6.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3t0e.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4euq.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4grl.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4h1l.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4may.pdb exists. Skipping
## download
```

```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4p4k.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4qrr.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4wuu.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4zez.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5brz.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5bs0.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5c07.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5c08.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5c09.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5c0a.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5c0b.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5c0c.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5e6i.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5e9d.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5eu6.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5euo.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5hhm.pdb exists. Skipping
## download
```

```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5hho.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5hyj.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5isz.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5jhd.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5jzi.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5ks9.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5ksa.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5ksb.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5men.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5nht.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5nme.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5nmf.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5nmg.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5nqk.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5tez.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5w1v.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5w1w.pdb exists. Skipping
## download
```

```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5wkf.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5wkh.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5xot.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5xov.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5yxn.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5yxu.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6am5.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6amu.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6avf.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6avg.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6bj2.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6bj3.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6bj8.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6cql.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6cqn.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6cqq.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6cqr.pdb exists. Skipping
## download
```

```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6d78.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6dfx.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6dkp.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6dxf.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6eqa.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6eqb.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6mtm.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6p64.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6px6.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6py2.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6q3s.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6r2l.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6rp9.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6rpa.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6rpb.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6rsy.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6tmo.pdb exists. Skipping
## download
```

```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6tro.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6u3n.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6u3o.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6uon.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6vm7.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6vm8.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6vma.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6vmc.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6vmx.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6vqo.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6vrm.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6vrn.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7n1e.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7n1f.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7n6e.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6xc9.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6xco.pdb exists. Skipping
## download
```

```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6xcp.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6zkw.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6zkx.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6zky.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6zkz.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7dzm.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7dzn.pdb exists. Skipping
## download

## Warning in download.file(get.files[k], put.files[k], quiet = !verbose):
## downloaded length 0 != reported length 260

## Warning in download.file(get.files[k], put.files[k], quiet = !verbose): cannot
## open URL 'https://files.rcsb.org/download/7ndq.pdb': HTTP status was '404 Not
## Found'

## Warning in file.remove(put.files[k]): cannot remove file 'tmp//7ndq.pdb',
## reason 'No such file or directory'

## Warning in download.file(get.files[k], put.files[k], quiet = !verbose):
## downloaded length 0 != reported length 260

## Warning in download.file(get.files[k], put.files[k], quiet = !verbose): cannot
## open URL 'https://files.rcsb.org/download/7ndu.pdb': HTTP status was '404 Not
## Found'

## Warning in file.remove(put.files[k]): cannot remove file 'tmp//7ndu.pdb',
## reason 'No such file or directory'

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7rm4.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7rtr.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7l1d.pdb exists. Skipping
## download
```

```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7sg0.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7sg1.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7sg2.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7rrg.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7n2s.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7n2n.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7n2o.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7n2r.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7n2p.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//7n2q.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//8cx4.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//8VCX.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//8VCY.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//8VD0.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//8VD2.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6XCP.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6XC0.pdb exists. Skipping
## download
```

```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6XC9.pdb exists. Skipping
## download

## Warning in get.pdb(pdb_ids, path = "tmp/"): Some files could not be downloaded,
## check returned value
```

```r
pdb_files <- pdb_files[endsWith(pdb_files, ".pdb")]
```

Align, superimpose and get coords. Then compute RMSD

```r
struct_alns <- pdbaln(pdb_files, fit = F,
                      ncore = 12,
                      exefile = "msa",
                      maxiters = 256)
```

```
## Reading PDB files:
## tmp//1ao7.pdb
## tmp//1bd2.pdb
## tmp//1fyt.pdb
## tmp//1j8h.pdb
## tmp//1mi5.pdb
## tmp//1oga.pdb
## tmp//1qrn.pdb
## tmp//1qse.pdb
## tmp//1qsf.pdb
## tmp//1zgl.pdb
## tmp//2ak4.pdb
## tmp//2bnq.pdb
## tmp//2bnr.pdb
## tmp//2esv.pdb
## tmp//2f53.pdb
## tmp//2f54.pdb
## tmp//2gj6.pdb
## tmp//2iam.pdb
## tmp//2ian.pdb
## tmp//2nx5.pdb
## tmp//2p5e.pdb
## tmp//2p5w.pdb
## tmp//2pye.pdb
## tmp//2vlj.pdb
## tmp//2vlk.pdb
## tmp//2vlr.pdb
## tmp//2xn9.pdb
## tmp//2ypl.pdb
## tmp//3d39.pdb
## tmp//3d3v.pdb
## tmp//3dxa.pdb
## tmp//3ffc.pdb
## tmp//3gsn.pdb
## tmp//3h9s.pdb
## tmp//3hg1.pdb
## tmp//3kpr.pdb
## tmp//3kps.pdb
```

```
## tmp//3kxf.pdb
## tmp//3mv7.pdb
## tmp//3mv8.pdb
## tmp//3mv9.pdb
## tmp//3o4l.pdb
## tmp//3pwp.pdb
## tmp//3qdg.pdb
## tmp//3qdj.pdb
## tmp//3qdm.pdb
## tmp//3qeq.pdb
## tmp//3qfj.pdb
## tmp//3sjv.pdb
## tmp//3uts.pdb
## tmp//3utt.pdb
## tmp//3vxm.pdb
## tmp//3vxr.pdb
## tmp//3vxs.pdb
## tmp//4c56.pdb
## tmp//4e41.pdb
## tmp//4eup.pdb
## tmp//4ftv.pdb
## tmp//4g8g.pdb
## tmp//4g9f.pdb
## tmp//4gg6.pdb
## tmp//4jfd.pdb
## tmp//4jfe.pdb
## tmp//4jff.pdb
## tmp//4jrx.pdb
## tmp//4jry.pdb
## tmp//4l3e.pdb
## tmp//4mji.pdb
## tmp//4mnq.pdb
## tmp//4ozf.pdb
## tmp//4ozg.pdb
## tmp//4ozh.pdb
## tmp//4ozi.pdb
## tmp//4prh.pdb
## tmp//4pri.pdb
## tmp//4prp.pdb
## tmp//4qok.pdb
## tmp//4qrp.pdb
## tmp//4y19.pdb
## tmp//4y1a.pdb
## tmp//4z7u.pdb
## tmp//4z7v.pdb
## tmp//4z7w.pdb
## tmp//5d2l.pdb
## tmp//5d2n.pdb
## tmp//1lp9.pdb
## tmp//1ymm.pdb
## tmp//2j8u.pdb
## tmp//2jcc.pdb
## tmp//2uwe.pdb
## tmp//2wbj.pdb
```

```
## tmp//3gjf.pdb
## tmp//3hae.pdb
## tmp//3nfj.pdb
## tmp//3o6f.pdb
## tmp//3pl6.pdb
## tmp//3t0e.pdb
## tmp//4euq.pdb
## tmp//4grl.pdb
## tmp//4h1l.pdb
## tmp//4may.pdb
## tmp//4p4k.pdb
## tmp//4qrr.pdb
## tmp//4wuu.pdb
## tmp//4zez.pdb
## tmp//5brz.pdb
## tmp//5bs0.pdb
## tmp//5c07.pdb
## tmp//5c08.pdb
## tmp//5c09.pdb
## tmp//5c0a.pdb
## tmp//5c0b.pdb
## tmp//5c0c.pdb
## tmp//5e6i.pdb
## tmp//5e9d.pdb
## tmp//5eu6.pdb
## tmp//5euo.pdb
## tmp//5hhm.pdb
## tmp//5hho.pdb
## tmp//5hyj.pdb
## tmp//5isz.pdb
## tmp//5jhd.pdb
## tmp//5jzi.pdb
## tmp//5ks9.pdb
## tmp//5ksa.pdb
## tmp//5ksb.pdb
## tmp//5men.pdb
## tmp//5nht.pdb
## tmp//5nme.pdb
## tmp//5nmf.pdb
## tmp//5nmg.pdb
## tmp//5nqk.pdb
## tmp//5tez.pdb
## tmp//5w1v.pdb
## tmp//5w1w.pdb
## tmp//5wkf.pdb
## tmp//5wkh.pdb
## tmp//5xot.pdb
## tmp//5xov.pdb
## tmp//5yxn.pdb
## tmp//5yxu.pdb
## tmp//6am5.pdb
## tmp//6amu.pdb
## tmp//6avf.pdb
## tmp//6avg.pdb
```

```
## tmp//6bj2.pdb
## tmp//6bj3.pdb
## tmp//6bj8.pdb
## tmp//6cql.pdb
## tmp//6cqn.pdb
## tmp//6cqq.pdb
## tmp//6cqr.pdb
## tmp//6d78.pdb
## tmp//6dfx.pdb
## tmp//6dkp.pdb
## tmp//6dxf.pdb
## tmp//6eqa.pdb
## tmp//6eqb.pdb
## tmp//6mtm.pdb
## tmp//6p64.pdb
## tmp//6px6.pdb
## tmp//6py2.pdb
## tmp//6q3s.pdb
## tmp//6r2l.pdb
## tmp//6rp9.pdb
## tmp//6rpa.pdb
## tmp//6rpb.pdb
## tmp//6rsy.pdb
## tmp//6tmo.pdb
## tmp//6tro.pdb
## tmp//6u3n.pdb
## tmp//6u3o.pdb
## tmp//6uon.pdb
## tmp//6vm7.pdb
## tmp//6vm8.pdb
## tmp//6vma.pdb
## tmp//6vmc.pdb
## tmp//6vmx.pdb
## tmp//6vqo.pdb
## tmp//6vrm.pdb
## tmp//6vrn.pdb
## tmp//7n1e.pdb
## tmp//7n1f.pdb
## tmp//7n6e.pdb
## tmp//6xc9.pdb
## tmp//6xco.pdb
## tmp//6xcp.pdb
## tmp//6zkw.pdb
## tmp//6zkx.pdb
## tmp//6zky.pdb
## tmp//6zkz.pdb
## tmp//7dzm.pdb
## tmp//7dzn.pdb
## tmp//7rm4.pdb
## tmp//7rtr.pdb
## tmp//7l1d.pdb
## tmp//7sg0.pdb
## tmp//7sg1.pdb
## tmp//7sg2.pdb
```

```
## tmp//7rrg.pdb
## tmp//7n2s.pdb
## tmp//7n2n.pdb
## tmp//7n2o.pdb
## tmp//7n2r.pdb
## tmp//7n2p.pdb
## tmp//7n2q.pdb
## tmp//8cx4.pdb
## tmp//8VCX.pdb
## tmp//8VCY.pdb
## tmp//8VD0.pdb
## tmp//8VD2.pdb
## tmp//6XCP.pdb
## tmp//6XC0.pdb
## tmp//6XC9.pdb
## .............  PDB has ALT records, taking A only, rm.alt=TRUE
## ..  PDB has ALT records, taking A only, rm.alt=TRUE
## .....  PDB has ALT records, taking A only, rm.alt=TRUE
## ..  PDB has ALT records, taking A only, rm.alt=TRUE
## .....  PDB has ALT records, taking A only, rm.alt=TRUE
##   PDB has ALT records, taking A only, rm.alt=TRUE
## ...  PDB has ALT records, taking A only, rm.alt=TRUE
## ..  PDB has ALT records, taking A only, rm.alt=TRUE
## ..  PDB has ALT records, taking A only, rm.alt=TRUE
## .  PDB has ALT records, taking A only, rm.alt=TRUE
## ..  PDB has ALT records, taking A only, rm.alt=TRUE
## ......  PDB has ALT records, taking A only, rm.alt=TRUE
## ....  PDB has ALT records, taking A only, rm.alt=TRUE
##   PDB has ALT records, taking A only, rm.alt=TRUE
## ..  PDB has ALT records, taking A only, rm.alt=TRUE
##   PDB has ALT records, taking A only, rm.alt=TRUE
## .  PDB has ALT records, taking A only, rm.alt=TRUE
## ...  PDB has ALT records, taking A only, rm.alt=TRUE
## ..  PDB has ALT records, taking A only, rm.alt=TRUE
## .  PDB has ALT records, taking A only, rm.alt=TRUE
## .  PDB has ALT records, taking A only, rm.alt=TRUE
##   PDB has ALT records, taking A only, rm.alt=TRUE
##   PDB has ALT records, taking A only, rm.alt=TRUE
## .  PDB has ALT records, taking A only, rm.alt=TRUE
##   PDB has ALT records, taking A only, rm.alt=TRUE
## ......  PDB has ALT records, taking A only, rm.alt=TRUE
## ...  PDB has ALT records, taking A only, rm.alt=TRUE
## .  PDB has ALT records, taking A only, rm.alt=TRUE
## ....  PDB has ALT records, taking A only, rm.alt=TRUE
## ..  PDB has ALT records, taking A only, rm.alt=TRUE
## ......  PDB has ALT records, taking A only, rm.alt=TRUE
## ....  PDB has ALT records, taking A only, rm.alt=TRUE
## ......  PDB has ALT records, taking A only, rm.alt=TRUE
## ......  PDB has ALT records, taking A only, rm.alt=TRUE
## .  PDB has ALT records, taking A only, rm.alt=TRUE
## ..  PDB has ALT records, taking A only, rm.alt=TRUE
## ........  PDB has ALT records, taking A only, rm.alt=TRUE
## ...  PDB has ALT records, taking A only, rm.alt=TRUE
## .  PDB has ALT records, taking A only, rm.alt=TRUE
```

```
##    PDB has ALT records, taking A only, rm.alt=TRUE
## ...   PDB has ALT records, taking A only, rm.alt=TRUE
## ............   PDB has ALT records, taking A only, rm.alt=TRUE
## .......   PDB has ALT records, taking A only, rm.alt=TRUE
##    PDB has ALT records, taking A only, rm.alt=TRUE
##    PDB has ALT records, taking A only, rm.alt=TRUE
## ......   PDB has ALT records, taking A only, rm.alt=TRUE
## ......   PDB has ALT records, taking A only, rm.alt=TRUE
##    PDB has ALT records, taking A only, rm.alt=TRUE
## ...   PDB has ALT records, taking A only, rm.alt=TRUE
## ..   PDB has ALT records, taking A only, rm.alt=TRUE
## .   PDB has ALT records, taking A only, rm.alt=TRUE
## ...   PDB has ALT records, taking A only, rm.alt=TRUE
## .   PDB has ALT records, taking A only, rm.alt=TRUE
## .   PDB has ALT records, taking A only, rm.alt=TRUE
## ..   PDB has ALT records, taking A only, rm.alt=TRUE
##    PDB has ALT records, taking A only, rm.alt=TRUE
## ....   PDB has ALT records, taking A only, rm.alt=TRUE
## ..   PDB has ALT records, taking A only, rm.alt=TRUE
## .   PDB has ALT records, taking A only, rm.alt=TRUE
## ..   PDB has ALT records, taking A only, rm.alt=TRUE
## ....   PDB has ALT records, taking A only, rm.alt=TRUE
## ....   PDB has ALT records, taking A only, rm.alt=TRUE
## .......   PDB has ALT records, taking A only, rm.alt=TRUE
##    PDB has ALT records, taking A only, rm.alt=TRUE
## .......   PDB has ALT records, taking A only, rm.alt=TRUE
## ..   PDB has ALT records, taking A only, rm.alt=TRUE
## .   PDB has ALT records, taking A only, rm.alt=TRUE
## .   PDB has ALT records, taking A only, rm.alt=TRUE
## ..   PDB has ALT records, taking A only, rm.alt=TRUE
## ...   PDB has ALT records, taking A only, rm.alt=TRUE
## ...   PDB has ALT records, taking A only, rm.alt=TRUE
## ..   PDB has ALT records, taking A only, rm.alt=TRUE
## ..   PDB has ALT records, taking A only, rm.alt=TRUE
## .   PDB has ALT records, taking A only, rm.alt=TRUE
## ........
##
## Extracting sequences
##
## pdb/seq: 1   name: tmp//1ao7.pdb
## pdb/seq: 2   name: tmp//1bd2.pdb
## pdb/seq: 3   name: tmp//1fyt.pdb
## pdb/seq: 4   name: tmp//1j8h.pdb
## pdb/seq: 5   name: tmp//1mi5.pdb
## pdb/seq: 6   name: tmp//1oga.pdb
## pdb/seq: 7   name: tmp//1qrn.pdb
## pdb/seq: 8   name: tmp//1qse.pdb
## pdb/seq: 9   name: tmp//1qsf.pdb
## pdb/seq: 10   name: tmp//1zgl.pdb
## pdb/seq: 11   name: tmp//2ak4.pdb
## pdb/seq: 12   name: tmp//2bnq.pdb
## pdb/seq: 13   name: tmp//2bnr.pdb
## pdb/seq: 14   name: tmp//2esv.pdb
## pdb/seq: 15   name: tmp//2f53.pdb
```

```
## pdb/seq: 17   name: tmp//2gj6.pdb
## pdb/seq: 16   name: tmp//2f54.pdb
## pdb/seq: 18   name: tmp//2iam.pdb
## pdb/seq: 19   name: tmp//2ian.pdb
## pdb/seq: 20   name: tmp//2nx5.pdb
## pdb/seq: 21   name: tmp//2p5e.pdb
## pdb/seq: 24   name: tmp//2vlj.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 25   name: tmp//2vlk.pdb
## pdb/seq: 26   name: tmp//2vlr.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 29   name: tmp//3d39.pdb
## pdb/seq: 27   name: tmp//2xn9.pdb
## pdb/seq: 30   name: tmp//3d3v.pdb
## pdb/seq: 33   name: tmp//3gsn.pdb
## pdb/seq: 36   name: tmp//3kpr.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 41   name: tmp//3mv9.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 42   name: tmp//3o4l.pdb
## pdb/seq: 28   name: tmp//2ypl.pdb
## pdb/seq: 45   name: tmp//3qdj.pdb
## pdb/seq: 39   name: tmp//3mv7.pdb
## pdb/seq: 37   name: tmp//3kps.pdb
## pdb/seq: 22   name: tmp//2p5w.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 23   name: tmp//2pye.pdb
## pdb/seq: 40   name: tmp//3mv8.pdb
## pdb/seq: 38   name: tmp//3kxf.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 49   name: tmp//3sjv.pdb
## pdb/seq: 53   name: tmp//3vxr.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 54   name: tmp//3vxs.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 51   name: tmp//3utt.pdb
## pdb/seq: 57   name: tmp//4eup.pdb
## pdb/seq: 48   name: tmp//3qfj.pdb
## pdb/seq: 34   name: tmp//3h9s.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 31   name: tmp//3dxa.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 32   name: tmp//3ffc.pdb
## pdb/seq: 35   name: tmp//3hg1.pdb
## pdb/seq: 52   name: tmp//3vxm.pdb
## pdb/seq: 65   name: tmp//4jrx.pdb
## pdb/seq: 66   name: tmp//4jry.pdb
## pdb/seq: 60   name: tmp//4g9f.pdb
## pdb/seq: 46   name: tmp//3qdm.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 47   name: tmp//3qeq.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 64   name: tmp//4jff.pdb
```

```
## pdb/seq: 77    name: tmp//4qok.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 69    name: tmp//4mnq.pdb
## pdb/seq: 78    name: tmp//4qrp.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 63    name: tmp//4jfe.pdb
## pdb/seq: 58    name: tmp//4ftv.pdb
## pdb/seq: 72    name: tmp//4ozh.pdb
## pdb/seq: 44    name: tmp//3qdg.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
##     PDB has ALT records, taking A only, rm.alt=TRUE
##     PDB has ALT records, taking A only, rm.alt=TRUE
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 59    name: tmp//4g8g.pdb
## pdb/seq: 89    name: tmp//2jcc.pdb
## pdb/seq: 76    name: tmp//4prp.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 81    name: tmp//4z7u.pdb
## pdb/seq: 43    name: tmp//3pwp.pdb
## pdb/seq: 61    name: tmp//4gg6.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 75    name: tmp//4pri.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 70    name: tmp//4ozf.pdb
## pdb/seq: 56    name: tmp//4e41.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 71    name: tmp//4ozg.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 88    name: tmp//2j8u.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 50    name: tmp//3uts.pdb
## pdb/seq: 84    name: tmp//5d2l.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 93    name: tmp//3hae.pdb
## pdb/seq: 55    name: tmp//4c56.pdb
## pdb/seq: 87    name: tmp//1ymm.pdb
## pdb/seq: 90    name: tmp//2uwe.pdb
## pdb/seq: 82    name: tmp//4z7v.pdb
## pdb/seq: 101   name: tmp//4may.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 73    name: tmp//4ozi.pdb
## pdb/seq: 99    name: tmp//4grl.pdb
## pdb/seq: 62    name: tmp//4jfd.pdb
## pdb/seq: 68    name: tmp//4mji.pdb
## pdb/seq: 83    name: tmp//4z7w.pdb
## pdb/seq: 113   name: tmp//5c0c.pdb
## pdb/seq: 100   name: tmp//4h1l.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 111   name: tmp//5c0a.pdb
## pdb/seq: 102   name: tmp//4p4k.pdb
## pdb/seq: 67    name: tmp//4l3e.pdb
```

```
## pdb/seq: 74    name: tmp//4prh.pdb
## pdb/seq: 94    name: tmp//3nfj.pdb
## pdb/seq: 85    name: tmp//5d2n.pdb
## pdb/seq: 112    name: tmp//5c0b.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 80    name: tmp//4y1a.pdb
## pdb/seq: 86    name: tmp//1lp9.pdb
## pdb/seq: 79    name: tmp//4y19.pdb
## pdb/seq: 95    name: tmp//3o6f.pdb
## pdb/seq: 125    name: tmp//5ksa.pdb
## pdb/seq: 96    name: tmp//3pl6.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 114    name: tmp//5e6i.pdb
## pdb/seq: 92    name: tmp//3gjf.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 105    name: tmp//4zez.pdb
## pdb/seq: 106    name: tmp//5brz.pdb
## pdb/seq: 123    name: tmp//5jzi.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 91    name: tmp//2wbj.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 108    name: tmp//5c07.pdb
## pdb/seq: 137    name: tmp//5wkh.pdb
## pdb/seq: 97    name: tmp//3t0e.pdb
## pdb/seq: 124    name: tmp//5ks9.pdb
## pdb/seq: 98    name: tmp//4euq.pdb
## pdb/seq: 107    name: tmp//5bs0.pdb
## pdb/seq: 118    name: tmp//5hhm.pdb
## pdb/seq: 109    name: tmp//5c08.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 104    name: tmp//4wuu.pdb
## pdb/seq: 117    name: tmp//5euo.pdb
## pdb/seq: 103    name: tmp//4qrr.pdb
## pdb/seq: 119    name: tmp//5hho.pdb
## pdb/seq: 149    name: tmp//6cql.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 120    name: tmp//5hyj.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 136    name: tmp//5wkf.pdb
## pdb/seq: 110    name: tmp//5c09.pdb
## pdb/seq: 130    name: tmp//5nmf.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 131    name: tmp//5nmg.pdb
## pdb/seq: 115    name: tmp//5e9d.pdb
## pdb/seq: 126    name: tmp//5ksb.pdb
## pdb/seq: 161    name: tmp//6px6.pdb
## pdb/seq: 135    name: tmp//5w1w.pdb
## pdb/seq: 116    name: tmp//5eu6.pdb
## pdb/seq: 129    name: tmp//5nme.pdb
## pdb/seq: 121    name: tmp//5isz.pdb
## pdb/seq: 173    name: tmp//6uon.pdb
## pdb/seq: 132    name: tmp//5nqk.pdb
##     PDB has ALT records, taking A only, rm.alt=TRUE
```

```
## pdb/seq: 127    name: tmp//5men.pdb
## pdb/seq: 148    name: tmp//6bj8.pdb
## pdb/seq: 128    name: tmp//5nht.pdb
## pdb/seq: 142    name: tmp//6am5.pdb
## pdb/seq: 122    name: tmp//5jhd.pdb
## pdb/seq: 143    name: tmp//6amu.pdb
## pdb/seq: 138    name: tmp//5xot.pdb
## pdb/seq: 144    name: tmp//6avf.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
##    PDB has ALT records, taking A only, rm.alt=TRUE
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 139    name: tmp//5xov.pdb
## pdb/seq: 133    name: tmp//5tez.pdb
## pdb/seq: 140    name: tmp//5yxn.pdb
## pdb/seq: 154    name: tmp//6dfx.pdb
## pdb/seq: 160    name: tmp//6p64.pdb
## pdb/seq: 141    name: tmp//5yxu.pdb
## pdb/seq: 155    name: tmp//6dkp.pdb
## pdb/seq: 185    name: tmp//6xc9.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 150    name: tmp//6cqn.pdb
## pdb/seq: 156    name: tmp//6dxf.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 152    name: tmp//6cqr.pdb
## pdb/seq: 145    name: tmp//6avg.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 167    name: tmp//6rpb.pdb
## pdb/seq: 162    name: tmp//6py2.pdb
## pdb/seq: 151    name: tmp//6cqq.pdb
## pdb/seq: 147    name: tmp//6bj3.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 166    name: tmp//6rpa.pdb
## pdb/seq: 153    name: tmp//6d78.pdb
## pdb/seq: 172    name: tmp//6u3o.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 168    name: tmp//6rsy.pdb
## pdb/seq: 134    name: tmp//5w1v.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 197    name: tmp//7sg0.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 174    name: tmp//6vm7.pdb
## pdb/seq: 159    name: tmp//6mtm.pdb
## pdb/seq: 164    name: tmp//6r2l.pdb
## pdb/seq: 157    name: tmp//6eqa.pdb
## pdb/seq: 178    name: tmp//6vmx.pdb
##    PDB has ALT records, taking A only, rm.alt=TRUE
##    PDB has ALT records, taking A only, rm.alt=TRUE
##    PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 165    name: tmp//6rp9.pdb
## pdb/seq: 209    name: tmp//8VCY.pdb
## pdb/seq: 163    name: tmp//6q3s.pdb
## pdb/seq: 171    name: tmp//6u3n.pdb
```

```
##      PDB has ALT records, taking A only, rm.alt=TRUE
##      PDB has ALT records, taking A only, rm.alt=TRUE
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 186   name: tmp//6xco.pdb
## pdb/seq: 184   name: tmp//7n6e.pdb
## pdb/seq: 169   name: tmp//6tmo.pdb
## pdb/seq: 176   name: tmp//6vma.pdb
## pdb/seq: 180   name: tmp//6vrm.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 190   name: tmp//6zky.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 179   name: tmp//6vqo.pdb
## pdb/seq: 175   name: tmp//6vm8.pdb
## pdb/seq: 183   name: tmp//7n1f.pdb
## pdb/seq: 181   name: tmp//6vrn.pdb
## pdb/seq: 198   name: tmp//7sg1.pdb
## pdb/seq: 188   name: tmp//6zkw.pdb
## pdb/seq: 192   name: tmp//7dzm.pdb
## pdb/seq: 195   name: tmp//7rtr.pdb
## pdb/seq: 187   name: tmp//6xcp.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 196   name: tmp//7l1d.pdb
## pdb/seq: 202   name: tmp//7n2n.pdb
## pdb/seq: 177   name: tmp//6vmc.pdb
## pdb/seq: 200   name: tmp//7rrg.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 204   name: tmp//7n2r.pdb
## pdb/seq: 193   name: tmp//7dzn.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 207   name: tmp//8cx4.pdb
## pdb/seq: 146   name: tmp//6bj2.pdb
## pdb/seq: 199   name: tmp//7sg2.pdb
## pdb/seq: 210   name: tmp//8VD0.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 208   name: tmp//8VCX.pdb
## pdb/seq: 189   name: tmp//6zkx.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 214   name: tmp//6XC9.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 212   name: tmp//6XCP.pdb
## pdb/seq: 191   name: tmp//6zkz.pdb
## pdb/seq: 205   name: tmp//7n2p.pdb
## pdb/seq: 158   name: tmp//6eqb.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 201   name: tmp//7n2s.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 203   name: tmp//7n2o.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 211   name: tmp//8VD2.pdb
## pdb/seq: 170   name: tmp//6tro.pdb
## pdb/seq: 213   name: tmp//6XC0.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
```

```
## pdb/seq: 182    name: tmp//7n1e.pdb
## pdb/seq: 194    name: tmp//7rm4.pdb
## pdb/seq: 206    name: tmp//7n2q.pdb
```

```r
# how coords are organized:
# (struct_alns$xyz |> matrix(nrow = 4))[1,] |> matrix(nrow = 3) |> t()
struct_alns_ids <- tools::file_path_sans_ext(basename(struct_alns$id))
struct_alns_coords <- struct_alns$xyz |>
  matrix(nrow = length(struct_alns$id)) |>
  t()
aligned_residues <- apply(struct_alns_coords, 2, \(x) sum(!is.na(x)))
struct_alns_coords[is.na(struct_alns_coords)] <- 0
# pairwise distances
struct_alns_eucl <- struct_alns_coords |>
  t() |>
  dist() |>
  as.matrix()
# normalize for number of aligned residues
struct_alns_rmsd <- t(struct_alns_eucl / sqrt(aligned_residues)) / sqrt(aligned_residues)
rownames(struct_alns_rmsd) <- struct_alns_ids
colnames(struct_alns_rmsd) <- struct_alns_ids
struct_alns_rmsd <- struct_alns_rmsd |>
  melt()
colnames(struct_alns_rmsd) <- c("clone_id.from", "clone_id.to", "rmsd")
summary(struct_alns_rmsd)
```

```
##  clone_id.from    clone_id.to         rmsd
##  1ao7   : 214   1ao7   : 214   Min.   :0.0000
##  1bd2   : 214   1bd2   : 214   1st Qu.:0.8535
##  1fyt   : 214   1fyt   : 214   Median :1.0666
##  1j8h   : 214   1j8h   : 214   Mean   :1.3506
##  1mi5   : 214   1mi5   : 214   3rd Qu.:1.4600
##  1oga   : 214   1oga   : 214   Max.   :8.1553
##  (Other):44512   (Other):44512
```

Plot RMSD, compare MHCI and MHCII - should be not much difference here due to gaps

```r
struct_alns_rmsd.mhc <- struct_alns_rmsd |>
  filter(clone_id.from != clone_id.to) |>
  left_join(vpdb_meta |>
              rename(mhc.from = mhc.class, clone_id.from = clone_id)) |>
  left_join(vpdb_meta |>
              rename(mhc.to = mhc.class, clone_id.to = clone_id))
```

```
## Joining with 'by = join_by(clone_id.from)'
## Joining with 'by = join_by(clone_id.to)'
```

```r
struct_alns_rmsd.mhc <-
  rbind(struct_alns_rmsd.mhc,
        struct_alns_rmsd.mhc |>
          mutate(mhc.tmp = mhc.from,
                 mhc.from = mhc.to,
```

```
                mhc.to = mhc.tmp)) |>
        select(-mhc.tmp)) |>
  unique()

ggplot(struct_alns_rmsd.mhc,
       aes(x = rmsd)) +
  geom_density(data = struct_alns_rmsd.mhc |>
                 select(rmsd),
               color = NA, fill = "#74add1") +
  geom_density(color = "black", fill = NA, size = 0.25) +
  facet_grid(mhc.from ~ mhc.to) +
  xlab("RMSD, Å") +
  ylab("Fraction of structure pairs") +
  theme_minimal() +
  theme(aspect.ratio = 1)
```
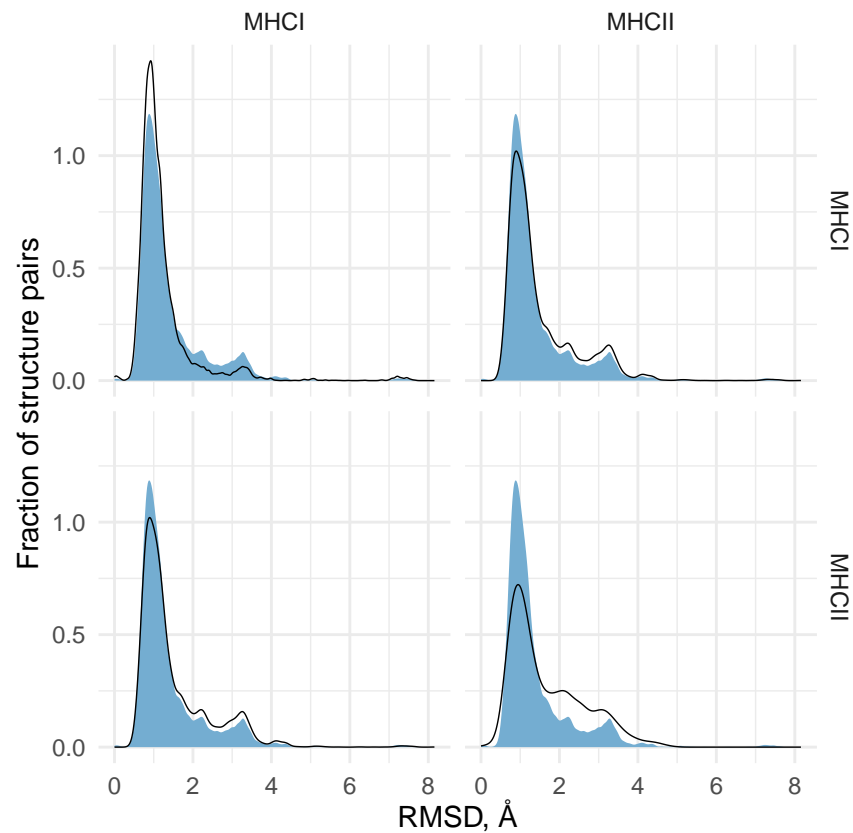
```
## Warning: Using 'size' aesthetic for lines was deprecated in ggplot2 3.4.0.
## i Please use 'linewidth' instead.
## This warning is displayed once every 8 hours.
## Call 'lifecycle::last_lifecycle_warnings()' to see where this warning was
## generated.
```


Distances from TCREMP

```
tcremp_dists <- read_tsv("v_tcrpmhc_tcremp.tsv")
```

```
## New names:
## Rows: 208 Columns: 1250
## -- Column specification
## ---------------------------------------------------------- Delimiter: "\t" chr
## (1): clone_id dbl (1249): ...1, 0_a_v, 0_a_j, 0_a_cdr3, 0_b_v, 0_b_j, 0_b_cdr3,
## 1_a_v, 1_a...
## i Use `spec()` to retrieve the full column specification for this data. i
## Specify the column types or set `show_col_types = FALSE` to quiet this message.
## * `` -> `...1`
```

```
fetch_dist <- function(dist_type) {
  tcremp_dists |>
    select(ends_with(dist_type)) |>
    as.matrix() ->
    mat
  rownames(mat) <- tcremp_dists$clone_id
  mat |>
    dist() |>
    as.matrix() |>
    melt(value.name = paste0("tcremp_", dist_type)) |>
    rename(clone_id.from = Var1, clone_id.to = Var2)
}

struct_alns_rmsd.mhc.dist <- struct_alns_rmsd.mhc |>
  left_join(fetch_dist("a_v")) |>
  left_join(fetch_dist("a_cdr3")) |>
  left_join(fetch_dist("a_j")) |>
  left_join(fetch_dist("b_v")) |>
  left_join(fetch_dist("b_cdr3")) |>
  left_join(fetch_dist("b_j"))
```

```
## Joining with `by = join_by(clone_id.from, clone_id.to)`
## Joining with `by = join_by(clone_id.from, clone_id.to)`
## Joining with `by = join_by(clone_id.from, clone_id.to)`
## Joining with `by = join_by(clone_id.from, clone_id.to)`
## Joining with `by = join_by(clone_id.from, clone_id.to)`
## Joining with `by = join_by(clone_id.from, clone_id.to)`
```

```
roundfactor <- 5.0
struct_alns_rmsd.mhc.dist |>
  melt(id.vars = 1:5,
       variable.name = "region",
       value.name = "distance") |>
  filter(clone_id.from > clone_id.to) |>
  mutate(chain = substr(region, 8, 8),
         rmsdr = round(rmsd * roundfactor, 0) / roundfactor) |>
  mutate(rmsdr = ifelse(rmsdr > 3, "4+", signif(rmsdr, 1)) |>
           as.factor()) |>
  ggplot(aes(x = rmsdr,
             group = rmsdr,
```

```
          y = distance,
          fill = chain)) +
geom_boxplot(alpha = 0.7, size = 0.3, outlier.size = 1.0,
             outlier.shape = "-") +
xlab("RMSD, Å") +
ylab("TCREMP distance") +
facet_wrap(. ~ region, scales = "free") +
scale_fill_brewer(guide = F, palette = "Set1") +
theme_minimal() +
theme(aspect.ratio = 1,
      axis.text.x = element_text(angle = 90, vjust = 0.5, hjust=1))
```
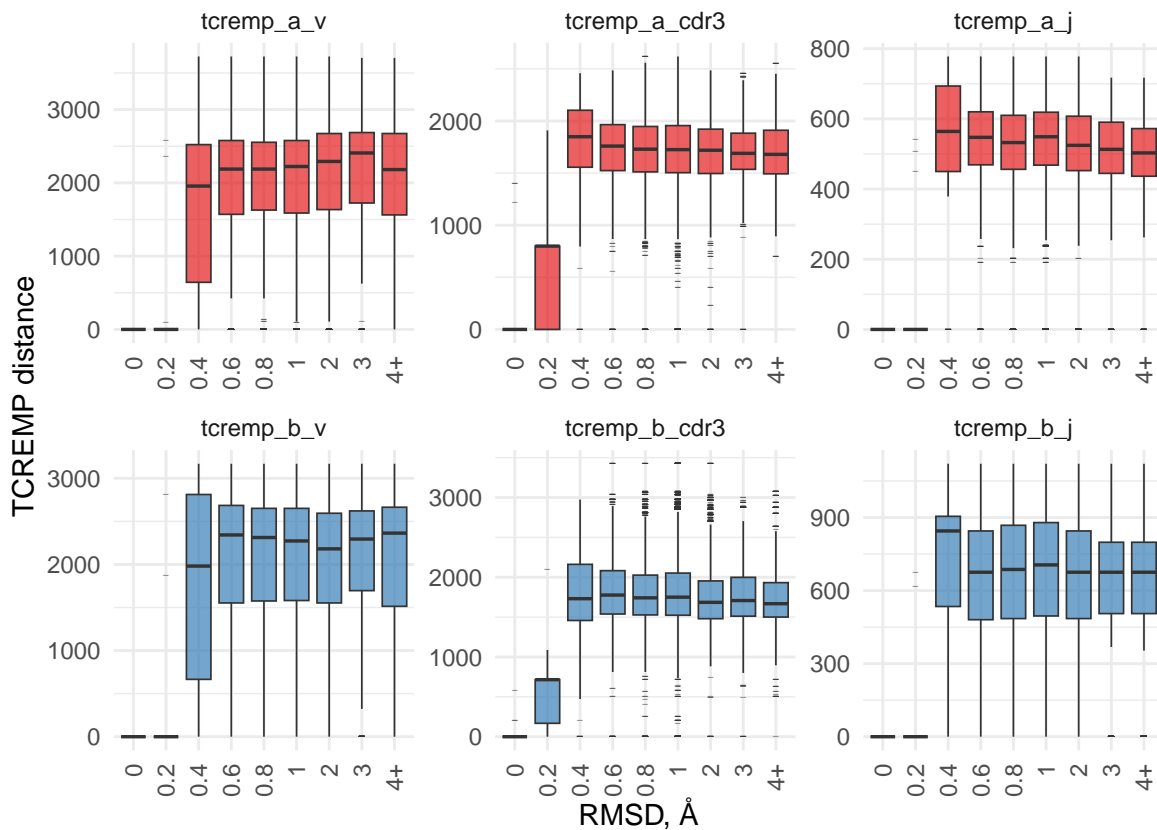
Warning: Removed 13206 rows containing non-finite outside the scale range
(`stat_boxplot()`).

Warning: The `guide` argument in `scale_*()` cannot be `FALSE`. This was deprecated in
ggplot2 3.3.4.
i Please use "none" instead.
This warning is displayed once every 8 hours.
Call `lifecycle::last_lifecycle_warnings()` to see where this warning was
generated.


```
#END
```