

# TCREMP and TCRpMHC structures

M.S.

2025-01-18

Fetch list of TCRs and their structures from VDJdb

```
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'
```

```
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> "CAVTTDSWGKLVF", "CAAMEGAQKLVF", "CAATGSFNKLVF", ~
## $ 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> "CASRPGLAGRPEQYF", "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, ~
## $ 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, ~
## $ 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.verifcation <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", "1fyf", "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", "1fyf", "1fyf", "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

```
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
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```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1qrn.pdb exists. Skipping
## download
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```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1qse.pdb exists. Skipping
## download
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```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1qsf.pdb exists. Skipping
## download
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## 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
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```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2bnr.pdb exists. Skipping
## download
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```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2esv.pdb exists. Skipping
## download
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```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2f53.pdb exists. Skipping
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```
## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2f54.pdb exists. Skipping
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```
## 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
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## 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
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3h9s.pdb exists. Skipping
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## 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
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## 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
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3qdj.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3qdm.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3qeq.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3qfj.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3sjv.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3uts.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3utt.pdb exists. Skipping
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## 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
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4g8g.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4g9f.pdb exists. Skipping
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## 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
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4jfe.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4jff.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4jrx.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4jry.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4l3e.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4mji.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4mnq.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4ozf.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4ozg.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4ozh.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4ozi.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4prh.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4qok.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4qrp.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4y19.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4y1a.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4z7u.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4z7v.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4z7w.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5d2l.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5d2n.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1lp9.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//1ymm.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2j8u.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2jcc.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2uwe.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//2wbj.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3gjf.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3hae.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//3t0e.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4euq.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4grl.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4h1l.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4may.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4p4k.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4qrr.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4wu0.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//4zez.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5brz.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5bs0.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5c07.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5c08.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5c09.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5c0a.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5c0b.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5c0c.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5e6i.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5e9d.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5eu6.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5euo.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5hbm.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5hho.pdb exists. Skipping
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## 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
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5jhd.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5jzi.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5ks9.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5ksa.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5ksb.pdb exists. Skipping
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5men.pdb exists. Skipping
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## 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
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//5nqk.pdb exists. Skipping
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## 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
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## 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
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## Warning in get.pdb(pdb_ids, path = "tmp/"): tmp//6cqr.pdb exists. Skipping
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## 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//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//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
```

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

Align, superimpose and get coords. Then compute RMSD

```
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//5hbm.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//6dxfl.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//6zxx.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



```

## .... 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: 19   name: tmp//2ian.pdb
## pdb/seq: 18   name: tmp//2iam.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: 26   name: tmp//2vlr.pdb
## pdb/seq: 25   name: tmp//2vlk.pdb
## pdb/seq: 27   name: tmp//2xn9.pdb
## pdb/seq: 29   name: tmp//3d39.pdb
## pdb/seq: 30   name: tmp//3d3v.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## 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 has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 41   name: tmp//3mv9.pdb
## pdb/seq: 42   name: tmp//3o4l.pdb
## pdb/seq: 28   name: tmp//2ypl.pdb
## pdb/seq: 39   name: tmp//3mv7.pdb
## pdb/seq: 37   name: tmp//3kps.pdb
## pdb/seq: 45   name: tmp//3qdj.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 has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 40   name: tmp//3mv8.pdb
## pdb/seq: 38   name: tmp//3kxf.pdb
## 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/seq: 48   name: tmp//3qfj.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 51   name: tmp//3utt.pdb
## pdb/seq: 34   name: tmp//3h9s.pdb
## pdb/seq: 32   name: tmp//3ffc.pdb
## pdb/seq: 31   name: tmp//3dxa.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 57   name: tmp//4eup.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## 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 has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 77 name: tmp//4qok.pdb
## PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 78 name: tmp//4qrp.pdb
## PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 44 name: tmp//3qdg.pdb
## pdb/seq: 72 name: tmp//4ozh.pdb
## pdb/seq: 63 name: tmp//4jfe.pdb
## pdb/seq: 58 name: tmp//4ftv.pdb
## pdb/seq: 69 name: tmp//4mnq.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: 76 name: tmp//4prp.pdb
## pdb/seq: 89 name: tmp//2jcc.pdb
## PDB has ALT records, taking A only, rm.alt=TRUE
## PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 43 name: tmp//3pwp.pdb
## PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 61 name: tmp//4gg6.pdb
## pdb/seq: 56 name: tmp//4e41.pdb
## pdb/seq: 75 name: tmp//4pri.pdb
## pdb/seq: 81 name: tmp//4z7u.pdb
## pdb/seq: 70 name: tmp//4ozf.pdb
## PDB has ALT records, taking A only, rm.alt=TRUE
## 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: 84 name: tmp//5d2l.pdb
## pdb/seq: 50 name: tmp//3uts.pdb
## PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 55 name: tmp//4c56.pdb
## pdb/seq: 87 name: tmp//1ymm.pdb
## pdb/seq: 90 name: tmp//2uwe.pdb
## pdb/seq: 93 name: tmp//3hae.pdb
## pdb/seq: 82 name: tmp//4z7v.pdb
## PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 101 name: tmp//4may.pdb
## PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 73 name: tmp//4ozi.pdb
## pdb/seq: 68 name: tmp//4mji.pdb
## pdb/seq: 99 name: tmp//4grl.pdb
## pdb/seq: 62 name: tmp//4jfd.pdb
## pdb/seq: 83 name: tmp//4z7w.pdb
## pdb/seq: 100 name: tmp//4h1l.pdb
## PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 113 name: tmp//5c0c.pdb
## pdb/seq: 67 name: tmp//4l3e.pdb
## pdb/seq: 111 name: tmp//5c0a.pdb
## pdb/seq: 102 name: tmp//4p4k.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: 79   name: tmp//4y19.pdb
## pdb/seq: 86   name: tmp//1lp9.pdb
## pdb/seq: 96   name: tmp//3pl6.pdb
## pdb/seq: 95   name: tmp//3o6f.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 125  name: tmp//5ksa.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/seq: 123  name: tmp//5jzi.pdb
## pdb/seq: 106  name: tmp//5brz.pdb
## pdb/seq: 91   name: tmp//2wbj.pdb
## pdb/seq: 108  name: tmp//5c07.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 105  name: tmp//4zez.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 97   name: tmp//3t0e.pdb
## pdb/seq: 137  name: tmp//5wkh.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 has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 104  name: tmp//4wuu.pdb
## pdb/seq: 103  name: tmp//4qrr.pdb
## pdb/seq: 109  name: tmp//5c08.pdb
## pdb/seq: 119  name: tmp//5hho.pdb
## pdb/seq: 120  name: tmp//5hyj.pdb
## pdb/seq: 117  name: tmp//5euo.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 149  name: tmp//6cql.pdb
## pdb/seq: 110  name: tmp//5c09.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 115  name: tmp//5e9d.pdb
## pdb/seq: 136  name: tmp//5wkf.pdb
## pdb/seq: 130  name: tmp//5nmf.pdb
## pdb/seq: 131  name: tmp//5nmg.pdb
## pdb/seq: 126  name: tmp//5ksb.pdb
## pdb/seq: 135  name: tmp//5w1w.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 116  name: tmp//5eu6.pdb
## pdb/seq: 161  name: tmp//6px6.pdb
## pdb/seq: 121  name: tmp//5isz.pdb
## pdb/seq: 132  name: tmp//5nqk.pdb
## pdb/seq: 129  name: tmp//5nme.pdb
## pdb/seq: 127  name: tmp//5men.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE

```



```

## pdb/seq: 128    name: tmp//5nht.pdb
## pdb/seq: 173    name: tmp//6uon.pdb
## pdb/seq: 148    name: tmp//6bj8.pdb
## pdb/seq: 122    name: tmp//5jhd.pdb
## pdb/seq: 142    name: tmp//6am5.pdb
## pdb/seq: 144    name: tmp//6avf.pdb
## pdb/seq: 143    name: tmp//6amu.pdb
## pdb/seq: 138    name: tmp//5xot.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 139    name: tmp//5xov.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 140    name: tmp//5yxn.pdb
## pdb/seq: 133    name: tmp//5tez.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 154    name: tmp//6dfx.pdb
## pdb/seq: 160    name: tmp//6p64.pdb
## pdb/seq: 155    name: tmp//6dkp.pdb
## pdb/seq: 156    name: tmp//6dxf.pdb
## pdb/seq: 150    name: tmp//6cqn.pdb
## pdb/seq: 141    name: tmp//5yxu.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 185    name: tmp//6xc9.pdb
## 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: 151    name: tmp//6cqq.pdb
## pdb/seq: 162    name: tmp//6py2.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: 168    name: tmp//6rsy.pdb
## pdb/seq: 172    name: tmp//6u3o.pdb
## pdb/seq: 153    name: tmp//6d78.pdb
## pdb/seq: 134    name: tmp//5w1v.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: 174    name: tmp//6vm7.pdb
## pdb/seq: 159    name: tmp//6mtm.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 197    name: tmp//7sg0.pdb
## pdb/seq: 164    name: tmp//6r2l.pdb
## pdb/seq: 157    name: tmp//6eqa.pdb
## pdb/seq: 178    name: tmp//6vmx.pdb
## pdb/seq: 163    name: tmp//6q3s.pdb
##      PDB has ALT records, taking A only, rm.alt=TRUE
## 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/seq: 186    name: tmp//6xco.pdb

```

```

## pdb/seq: 165   name: tmp//6rp9.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 209   name: tmp//8VCY.pdb
## pdb/seq: 180   name: tmp//6vrm.pdb
## pdb/seq: 184   name: tmp//7n6e.pdb
## pdb/seq: 176   name: tmp//6vma.pdb
## pdb/seq: 169   name: tmp//6tmo.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 175   name: tmp//6vm8.pdb
## pdb/seq: 190   name: tmp//6zky.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 183   name: tmp//7n1f.pdb
## pdb/seq: 179   name: tmp//6vqo.pdb
## pdb/seq: 198   name: tmp//7sg1.pdb
## pdb/seq: 181   name: tmp//6vrn.pdb
## pdb/seq: 192   name: tmp//7dzm.pdb
## pdb/seq: 188   name: tmp//6zkw.pdb
## pdb/seq: 187   name: tmp//6xcp.pdb
## pdb/seq: 195   name: tmp//7rtr.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 202   name: tmp//7n2n.pdb
## pdb/seq: 204   name: tmp//7n2r.pdb
## pdb/seq: 196   name: tmp//7l1d.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 200   name: tmp//7rrg.pdb
## pdb/seq: 177   name: tmp//6vmc.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 207   name: tmp//8cx4.pdb
## pdb/seq: 199   name: tmp//7sg2.pdb
## pdb/seq: 193   name: tmp//7dzn.pdb
## pdb/seq: 146   name: tmp//6bj2.pdb
## pdb/seq: 210   name: tmp//8VD0.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: 214   name: tmp//6XC9.pdb
## pdb/seq: 208   name: tmp//8VCX.pdb
## pdb/seq: 189   name: tmp//6zqx.pdb
## pdb/seq: 212   name: tmp//6XCP.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## 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/seq: 211   name: tmp//8VD2.pdb
## 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 has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 170   name: tmp//6tro.pdb
##   PDB has ALT records, taking A only, rm.alt=TRUE
## pdb/seq: 213   name: tmp//6XC0.pdb

```

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

```
# 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
## 1fyf : 214 1fyf : 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

```
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)'
```

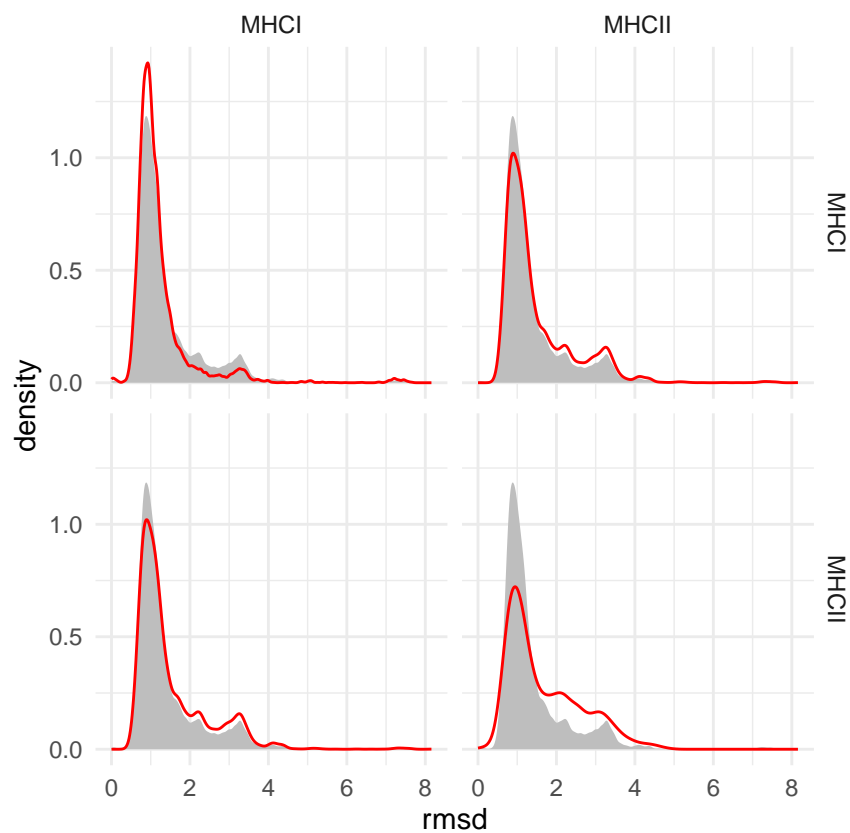
```
struct_alns_rmsd.mhc <-
  rbind(struct_alns_rmsd.mhc,
    struct_alns_rmsd.mhc |>
      mutate(mhc.tmp = mhc.from,
        mhc.from = mhc.to,
```

```

      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 = "grey") +
  geom_density(color = "red", fill = NA) +
  facet_grid(mhc.from ~ mhc.to) +
  theme_minimal() +
  theme(aspect.ratio = 1)

```



#END