

Characterizing Heme Pockets



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For those who gave me inspiration but now give never more

Acknowledgements

In case anyone reads this in the future, some context may be appreciated: I attended and completed this Master's during the COVID-19 global pandemic from September 2020 to September 2021.

Thanks professors

Thanks lab

Thanks UAB

Thanks Spain, and Catalonia, allowing me in and then also having public health measures unlike Donny's America

Thanks classmates

Thanks fam, friends

Thanks to the media and the creators of media that facilitated the survival of my sanity through the pandemic.

Finally, I'd like to quote a well-known artist from California. He was referencing his own work, but I wholly identify with his appreciation for the subject of his esteem:

“Last but not least, I wanna thank me. I wanna thank me for believing in me. I wanna thank me for doing all this hard work. I wanna thank me for having no days off. I wanna thank me for, for never quitting. I wanna thank me for always being a giver, and trying to give more than I receive. I wanna thank me for trying to do more right than wrong. I wanna thank me for just being me at all times.” – Calvin Cordozar Broadus Jr.

Abstract

Metalloproteins compose approximately 40 percent (look up how to do percents in latex) of all known proteins, and use some metallic group to accomplish their chemistry. One such metallic group is heme. Heme is a member of the porphyrin family, which are able to catalyze a broad range of reactions. Heme in particular catalyzes many different reactions and is present in many proteins. However, the underlying structural requirements to host heme in a protein are not well studied.

In this study, all heme or heme-c containing proteins as of xx were downloaded and processed in order to determine underlying structural characteristics these proteins may have in common. Parameters that were examined include: xx. Overall, we found: xx. These results may have implications for protein engineering; or if I fucked up this illustrates the difficulty of the field and demonstrate the wide range of acceptable environments of heme; it may therefore be more appropriate to take a more hands-on approach until perhaps other computational methods evolve to better examine structure-function relationships.

See? Not so bad of a worst-case scenario. Just, an unusual sentiment to see in modern science.

Contents

List of Figures	vii
List of Tables	viii
List of Abbreviations	ix
Lay Summary	1
Introduction	2
1 How to use	4
1.1 How <code>oxforddown</code> is structured	4
1.2 Building your entire thesis	8
1.3 Building a single chapter	10
2 R Markdown basics	12
2.1 Basic markdown syntax	13
2.2 Executable code chunks	17
2.3 Executable inline code	22
2.4 Executable code in other languages than R	23
3 Citations, cross-references, and collaboration	24
3.1 Citations	24
3.2 Cross-referencing	27
3.3 Collaborative writing	30
3.4 Additional resources	31
4 Tables	32
4.1 Making LaTeX tables play nice	32

5	Customisations and extensions	46
5.1	Front matter	47
5.2	Shorten running header (PDF)	48
5.3	Unnumbered chapters	48
5.4	Beginning chapters with quotes (PDF)	48
5.5	Highlighting corrections (HTML & PDF)	49
5.6	Apply custom font color and highlighting to text (HTML & PDF) .	50
5.7	Including another paper in your thesis - embed a PDF document . .	51
5.8	Including another paper in your thesis - R Markdown child document	55
5.9	Customizing referencing	59
5.10	Customizing the page headers and footers (PDF)	62
5.11	Diving in to the OxThesis LaTeX template (PDF)	63
5.12	Customising to a different university	63
6	Troubleshooting	65
6.1	Error: Failed to build the bibliography via biber	65
	Conclusion	67
	More info	67
7	Methods	68
7.1	Datasets	68
8	Results	69
	Trial	70
	Appendices	
A	Figures	72
A.1	AA Frequency	72
B	Tables	83
B.1	Molecule Names and Source Organisms	83
	Works Cited	89

List of Figures

2.1	Code chunk syntax	17
2.2	Oxford logo	19
2.3	Oxford logo, rotated	20
2.4	A ggplot of car stuff	20
2.5	An Oxford logo that LaTeX will try to place at this position in the text	22
3.1	The ‘citr’ add-in	27
3.2	A marvel-lous meme	29
4.1	Font sizes in LaTeX	43
A.1	HEM: AA Frequency	73
A.2	HEM: Volume	74
A.3	HEM: Ligand Excluded Surface Area	75
A.4	HEM: Ligand Accessible Surface Area	76
A.5	HEM: Pocket Excluded Surface Area	77
A.6	HEM: Pocket Accessible Surface Area	78
A.7	HEM: All Planar Angles	79
A.8	HEM: Planar Angles of Closest Residues	80
A.9	HEM: All CACBFe Angles	81
A.10	HEM: Closest CACBFe Angles	82

List of Tables

2.1	A knitr kable table	21
3.1	Stopping cars	29
B.1	HEMp1DF	83
B.2	HEMp2DF	87

List of Abbreviations

- 1-D, 2-D** . . . One- or two-dimensional, referring **in this thesis** to spatial dimensions in an image.
- Otter** One of the finest of water mammals.
- Hedgehog** . . . Quite a nice prickly friend.

Lay Summary

I investigated how heme, a molecule involved in many biological processes, binds to proteins. I did this by...

Introduction

Proteins may catalyze reactions, and many require ligands to enable their chemistry. A significant portion of all proteins, approximately 40%, require a metallic group as a ligand in order to function correctly - these proteins are known as metalloproteins.

One of these metallic groups is heme. Heme is a member of the porphyrin family, a group of molecules capable of catalyzing a broad range of reactions. Heme can catalyze many different reactions and is present in many proteins. However, the underlying structural requirements to host heme in a protein are not well understood. [MAY ADD CITATIONS]

There have only been a handful of studies dedicated to understanding the structure-chemical relationship between heme and the proteins that use heme for their chemistry (these proteins are known as hemoproteins).

In the most significant previous work, approximately ~125 hemoproteins were studied (Li et al. [1]). Although pdbs were thoroughly examined and the datasets were culled, the sample size of this study is very small compared to the amount of hemoproteins available in the pdb a decade later (~10,000 HEM-containing proteins and xx). The dataset is also limited in that there is a somewhat homogenous group of proteins examined (?). The characteristics examined were limited to: xx.

It is hypothesized that the following characteristics all have an impact on the binding of heme and function of the hemoprotein: XXXXXXXXXX.

In this study, some of these characteristics were examined. They include: XX. The remainder are thus far not feasible to calculate.

All of these characteristics have implications in the field of protein engineering or basic research into hemoproteins. Examples of the uses of these results include [SUPER BLOOD STUDY] and [OTHER PROTEIN ENGINEERING STUFF]. Not

Introduction

sure how much we can reference those other papers besides doing that besides in the conclusion.

Notable results from some of the prior studies include: xx and xx. These characteristics are also examined in this dataset, while some are not due to different study approaches.

1

How to use

Contents

1.1	How <code>oxforddown</code> is structured	4
1.1.1	<code>index.Rmd</code> : metadata and layout options	5
1.1.2	other .Rmd files in root folder: thesis chapters	7
1.1.3	front-and-back-matter/	7
1.1.4	<code>_bookdown.yml</code> : build options	7
1.1.5	scripts-and-filters	8
1.1.6	templates	8
1.2	Building your entire thesis	8
1.3	Building a single chapter	10

1.1 How `oxforddown` is structured

```
.
+-- index.Rmd
+-- _bookdown.yml
+-- 00-introduction.Rmd
|   ...
+-- 07-conclusion.Rmd
+-- front-and-back-matter
```

1. How to use

```
|   +-- _abstract.Rmd
|   +-- 98-appendices.Rmd
|   ...
+-- bibliography
|   +-- references.bib
|   ...
+-- figures
|   ...
+-- docs
|   +-- _main.pdf
|   ...
+-- scripts_and_filters
|   +-- knit-functions.R
|   ...
+-- templates
|   +-- template.tex
|   ...
```

1.1.1 index.Rmd: metadata and layout options

In index.Rmd, set your thesis' basic metadata (e.g., title, author name)

```
title: |
  `oxforddown`: \
  An Oxford University Thesis \
  Template for R Markdown
author: Author Name
college: Your College
```

Also set filepath(s) to your abstract, acknowledgements, abbreviations, and bibliography (one or more **.bib** files):

1. How to use

```
abstract: |
  `r paste(readLines("front-and-back-matter/_abstract.Rmd"), collapse = '\n ')`
acknowledgements: |
  `r paste(readLines("front-and-back-matter/_acknowledgements.Rmd"), collapse = '\n ')`
dedication: For Yihui Xie
abbreviations: |
  `r paste(readLines("front-and-back-matter/_abbreviations.Rmd"), collapse = '\n ')`

#####
## bibliography path ##
#####
bibliography: [bibliography/references.bib, bibliography/additional-references.bib]
```

Finally, **index.Rmd** is also where you customise layout options. For example, in PDF output what should the heading for the bibliography section say? How should page numbers be positioned? Should line numbers be shown? In HTML output, what CSS files should be used for styling?

```
### citation and bibliography style ###
bibliography-heading-in-pdf: Works Cited
...

### position of page numbers ###
ordinary-page-number-foot-or-head: foot #'foot' puts page number in footer, 'head' in header
ordinary-page-number-position: C
...

includeline-num: false #show line numbering in PDF?
...

bookdown::bs4_book:
```

1. How to use

css:

- *templates/bs4_style.css*
- *templates/corrections.css # remove to stop highlighting corrections*

1.1.2 other .Rmd files in root folder: thesis chapters

- each chapter of your thesis should have its own **.Rmd** file in the root directory
- when you knit **index.Rmd**, these chapters are merged together in alphabetical order, based on their filenames

1.1.3 front-and-back-matter/

- this folder holds the front and back matter of your thesis
- it has **.Rmd** files for your abstract, acknowledgements, abbreviations, and a welcome note that is included in HTML output. Note how these files start with an underscore (e.g. **__abstract.Rmd**). This means they will not automatically be merged into the thesis – they are explicitly included in **index.Rmd**
- **98-appendices** and **99-references.Rmd** are automatically merged into thesis, however - therefore their file names start with a high number, so that they will be included by the very end (merging is done alphabetically)
- **99-references.Rmd** sole purpose is to set the heading for the references section in HTML and Word output

1.1.4 __bookdown.yml: build options

- Set output directory for your thesis files (**docs/** is the default, as it makes it easy to publish HTML output on GitHub pages)
- Should R Markdown automatically merge **.Rmd** files in alphabetical order? Alternatively, specify explicitly which files should be included.

1. How to use

1.1.5 scripts-and-filters

- **knit-function.R** has the functions that are used when you build the entire thesis by knitting **index.Rmd**
- **create_chunk_options.R** lets you include cute quotes at the start of a chapter in PDF output
- **colour_and_highlight.lua** lets you color text or apply background color to text

1.1.6 templates

- **template.tex** is the LaTeX template used to build the entire thesis to PDF in the OxThesis layout (relies on **ociamthesis.cls**)
- **brief-template.tex** is the LaTeX template used to build a single chapter to PDF in the OxThesis layout (relies on **ociamthesis.cls**)
- **beltcrest.pdf**: the oxford logo used on the front page of the PDF output

1.2 Building your entire thesis

- Build the entire thesis by opening **index.Rmd** and clicking the ‘knit’ button.
- The generated thesis files are saved in the **docs/** folder
- To choose output formats, go to the top of **index.Rmd**’s YAML header and edit the line `thesis_formats <- "pdf"`; to the format(s) you want (options are “pdf”, “bs4”, “gitbook”, and “word”)
- You can build to multiple formats simultaneously with, e.g., `thesis_formats <- c("pdf", "bs4", "word")`
- If you want to customise the build function, edit **scripts_and_filters/knit-functions.R**

1. How to use

PDF output

```
knit: (function(input, ...) {  
  thesis_formats <- "pdf";  
  ...  
})
```

When you build the entire thesis to PDF, Latex generates a whole bunch of auxillary files - these are automatically removed after the build process end by the custom knit function that is used when you knit **index.Rmd**.

To change how this removal is done, edit **scripts__and__filters/knit-functions.R**.

The line `file.remove(list.files(pattern = "*\\.(log|mtc\\d*|maf|aux|bcf|lof|lot|out|t` within `if ("pdf" %in% output_format){` is the one that removes files after PDF output is generated.

BS4 book output (HTML)

```
knit: (function(input, ...) {  
  thesis_formats <- "bs4";  
  ...  
})
```

- NOTE: the [bs4 book output](#) requires the `downlit` and `bslib` R packages (install them with `install.packages`)
- Note also that to deploy a BS4 book on GitHub Pages, there must be a **.nojekyll** file in the **docs/** folder, otherwise GitHub does some voodoo that causes some filepaths not to work. This file is generated automatically by `oxforddowns` knitting function.

Gitbook output (HTML)

```
knit: (function(input, ...) {  
  thesis_formats <- "gitbook";  
  ...  
})
```

1. How to use

- Note that to deploy a gitbook on GitHub Pages, there must be a **.nojekyll** file in the **docs/** folder, otherwise GitHub does some voodoo that causes some filepaths not to work. This file is generated automatically by **oxforddowns** knitting function.

Word output

```
knit: (function(input, ...) {  
  thesis_formats <- "word";  
  ...  
})
```

- Note that the Word output has no templates behind it, and many things do not work (e.g. image rotation, highlighting corrections). **I encourage pull requests that optimise the Word output, e.g. by using tools from the **officer** package.**

1.3 Building a single chapter

To knit an individual chapter without compiling the entire thesis you:

1. open the **.Rmd** file of a chapter
2. add a YAML header specifying the output format(s) (e.g. **bookdown::word_document2** for a word document you might want to upload to Google Docs for feedback from collaborators)
3. click the **knit** button (the output file is then saved in the root folder)

As shown in the sample chapters' YAML headers, to output a single chapter to PDF, use e.g.:

```
output:  
  bookdown::pdf_document2:  
    template: templates/brief_template.tex  
    citation_package: biblatex
```

1. How to use

```
documentclass: book  
bibliography: references.bib
```

The file **templates/brief_template.tex** formats the chapter in the OxThesis style but without including the front matter (table of contents, abstract, etc).

Neque porro quisquam est qui dolorem ipsum quia dolor sit amet, consectetur, adipisci velit...

There is no one who loves pain itself, who seeks after it and wants to have it, simply because it is pain...

— Cicero's *de Finibus Bonorum et Malorum*.

2

R Markdown basics

Contents

2.1	Basic markdown syntax	13
2.1.1	Whitespace	13
2.1.2	Italics and bold	13
2.1.3	Inline code	13
2.1.4	Sub and superscript	13
2.1.5	Strikethrough	13
2.1.6	'Escaping' (aka "What if I need an actual asterisk?") . .	14
2.1.7	Endash (–), emdash (—)	14
2.1.8	Blockquotes	14
2.1.9	Headings	14
2.1.10	Lists	14
2.1.11	Line breaks	15
2.1.12	Hyperlinks	15
2.1.13	Footnotes	16
2.1.14	Comments	16
2.1.15	Math	16
2.2	Executable code chunks	17
2.2.1	Setup chunks - setup, images, plots	18
2.2.2	Including images	18
2.2.3	Including plots	19
2.2.4	Including tables	21
2.2.5	Control positioning	21
2.3	Executable inline code	22
2.4	Executable code in other languages than R	23

Here is a brief introduction to using *R Markdown*. *Markdown* is a simple formatting

2. *R Markdown basics*

syntax for authoring HTML, PDF, and MS Word documents and much, much more. *R Markdown* provides the flexibility of *Markdown* with the implementation of **R** input and output. For more details on using *R Markdown* see <http://rmarkdown.rstudio.com>.

2.1 Basic markdown syntax

2.1.1 Whitespace

Be careful with your spacing. While whitespace largely is ignored, it does at times give markdown signals as to how to proceed. As a habit, try to keep everything left aligned whenever possible, especially as you type a new paragraph. In other words, there is no need to indent basic text in the Rmd document (in fact, it might cause your text to do funny things if you do).

2.1.2 Italics and bold

- *Italics* are done like **this** or *__this__*
- **Bold** is done like ****this**** or **___this___**
- ***Bold and italics*** is done like *****this*****, **_____this_____**, or (the most transparent solution, in my opinion) ****_this_****

2.1.3 Inline code

- Inline code is created with backticks like ``this``

2.1.4 Sub and superscript

Sub₂ and super² script is created like this~2~ and this^2^

2.1.5 Strikethrough

- ~~Strikethrough~~ is done ~like this~

2.1.6 ‘Escaping’ (aka “What if I need an actual asterisk?”)

- To include an actual *, _ or \, add another \ in front of them: *, _, \\

2.1.7 Endash (–), emdash (—)

- – and — with -- and ---

2.1.8 Blockquotes

Do like this:

Put a > in front of the line.

2.1.9 Headings

Section headers are created with #’s of increasing number, i.e.

- # First-level heading
- ## Second-level heading
- ### Etc.

In PDF output, a level-five heading will turn into a paragraph heading, i.e. `\paragraph{My level-five heading}`, which appears as bold text on the same line as the subsequent paragraph.

2.1.10 Lists

Unordered list by starting a line with an * or a -:

- Item 1
- Item 2

Ordered lists by starting a line with a number. Notice that you can mislabel the numbers and *Markdown* will still make the order right in the output:

1. Item 1

2. *R Markdown basics*

2. Item 2

To create a sublist, indent the values a bit (at least four spaces or a tab):

1. Item 1
2. Item 2
3. Item 3
 - Item 3a
 - Item 3b

2.1.11 Line breaks

The official *Markdown* way to create line breaks is by ending a line with more than two spaces.

Roses are red. Violets are blue.

This appears on the same line in the output, because we didn't add spaces after red.

Roses are red.

Violets are blue.

This appears with a line break because I added spaces after red.

I find this is confusing, so I recommend the alternative way: Ending a line with a backslash will also create a linebreak:

Roses are red.

Violets are blue.

To create a new paragraph, you put a blank line.

Therefore, this line starts its own paragraph.

2.1.12 Hyperlinks

- [This is a hyperlink](#) created by writing the text you want turned into a clickable link in [square brackets followed by a](https://hyperlink-in-parentheses)

2.1.13 Footnotes

- Are created¹ by writing either `^[my footnote text]` for supplying the footnote content inline, or something like `[^a-random-footnote-label]` and supplying the text elsewhere in the format shown below ²:

`[^a-random-footnote-label]: This is a random test.`

2.1.14 Comments

To write comments within your text that won't actually be included in the output, use the same syntax as for writing comments in HTML. That is, `<!-- this will not be included in the output -->`.

2.1.15 Math

The syntax for writing math is stolen from LaTeX. To write a math expression that will be shown **inline**, enclose it in dollar signs. - This: `$A = \pi*r^{2}$`
Becomes: $A = \pi * r^2$

To write a math expression that will be shown in a block, enclose it in two dollar signs.

This: `$$A = \pi*r^{2}$$`

Becomes:

$$A = \pi * r^2$$

To create numbered equations, put them in an 'equation' environment and give them a label with the syntax `(\#eq:label)`, like this:

```
\begin{equation}
  f\left(k\right) = \binom{n}{k} p^k\left(1-p\right)^{n-k}
  (\#eq:binom)
\end{equation}
```

¹my footnote text

²This is a random test.

2. R Markdown basics

Becomes:

$$f(k) = \binom{n}{k} p^k (1-p)^{n-k} \quad (2.1)$$

For more (e.g. how to theorems), see e.g. the documentation on bookdown.org

2.2 Executable code chunks

The magic of R Markdown is that we can add executable code within our document to make it dynamic.

We do this either as *code chunks* (generally used for loading libraries and data, performing calculations, and adding images, plots, and tables), or *inline code* (generally used for dynamically reporting results within our text).

The syntax of a code chunk is shown in Figure 2.1.

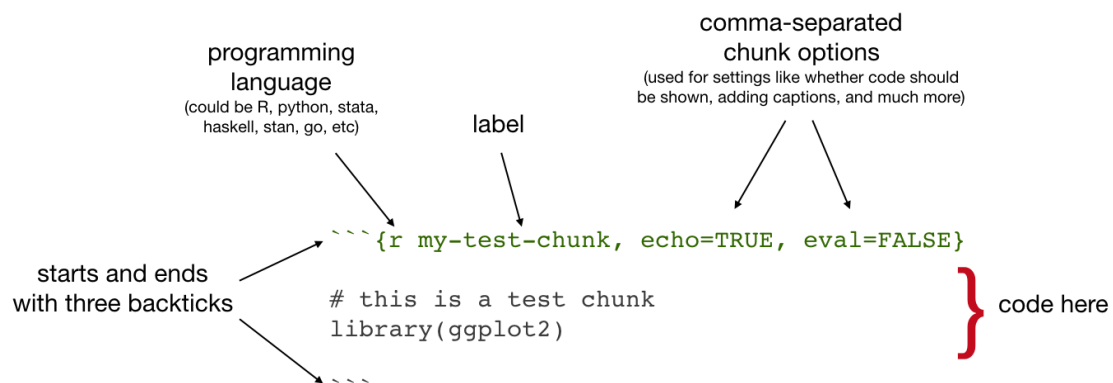


Figure 2.1: Code chunk syntax

Common chunk options include (see e.g. bookdown.org):

- **echo**: whether or not to display code in knitted output
- **eval**: whether or not to run the code in the chunk when knitting
- **include**: whether to include anything from the from a code chunk in the output document
- **fig.cap**: figure caption
- **fig.scap**: short figure caption, which will be used in the ‘List of Figures’ in the PDF front matter

IMPORTANT: Do *not* use underscores in your chunk labels - if you do, you are likely to get an error in PDF output saying something like “! Package caption Error: \caption outside float”.

2.2.1 Setup chunks - setup, images, plots

An R Markdown document usually begins with a chunk that is used to **load libraries**, and to **set default chunk options** with `knitr::opts_chunk$set`.

In your thesis, this will probably happen in **index.Rmd** and/or as opening chunks in each of your chapters.

```
““{r setup, include=FALSE}
# don't show code unless we explicitly set echo = TRUE
knitr::opts_chunk$set(echo = FALSE)

library(tidyverse)
““
```

2.2.2 Including images

Code chunks are also used for including images, with `include_graphics` from the `knitr` package, as in [Figure 2.2](#)

```
knitr::include_graphics("figures/sample-content/beltcrest.png")
```

Useful chunk options for figures include:

- `out.width` (use with a percentage) for setting the image size
- if you’ve got an image that gets waaay to big in your output, it will be constrained to the page width by setting `out.width = "100%"`

Figure rotation

You can use the chunk option `out.extra` to rotate images.

The syntax is different for LaTeX and HTML, so for ease we might start by assigning the right string to a variable that depends on the format you’re outputting to:



Figure 2.2: Oxford logo

```
if (knitr::is_latex_output()){  
  rotate180 <- "angle=180"  
} else {  
  rotate180 <- "style='transform:rotate(180deg);'"  
}
```

Then you can reference that variable as the value of `out.extra` to rotate images, as in Figure 2.3.

2.2.3 Including plots

Similarly, code chunks are used for including dynamically generated plots. You use ordinary code in R or other languages - Figure 2.4 shows a plot of the `cars` dataset of stopping distances for cars at various speeds (this dataset is built in to **R**).

```
cars %>%  
  ggplot() +  
    aes(x = speed, y = dist) +  
    geom_point()
```

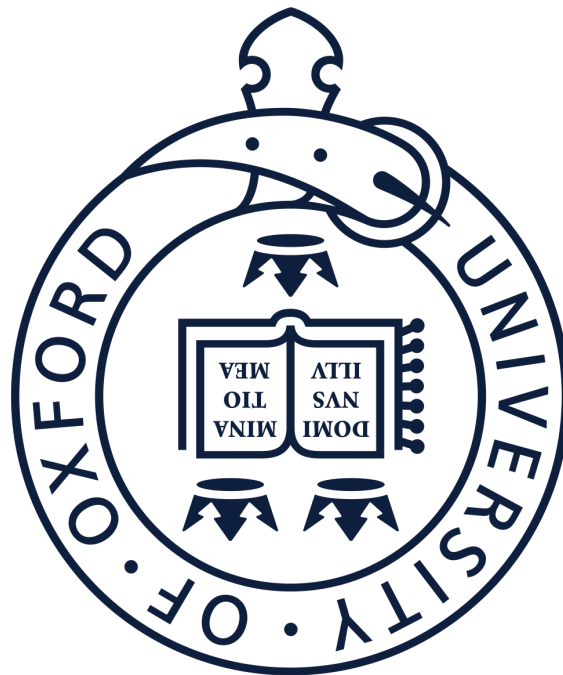


Figure 2.3: Oxford logo, rotated

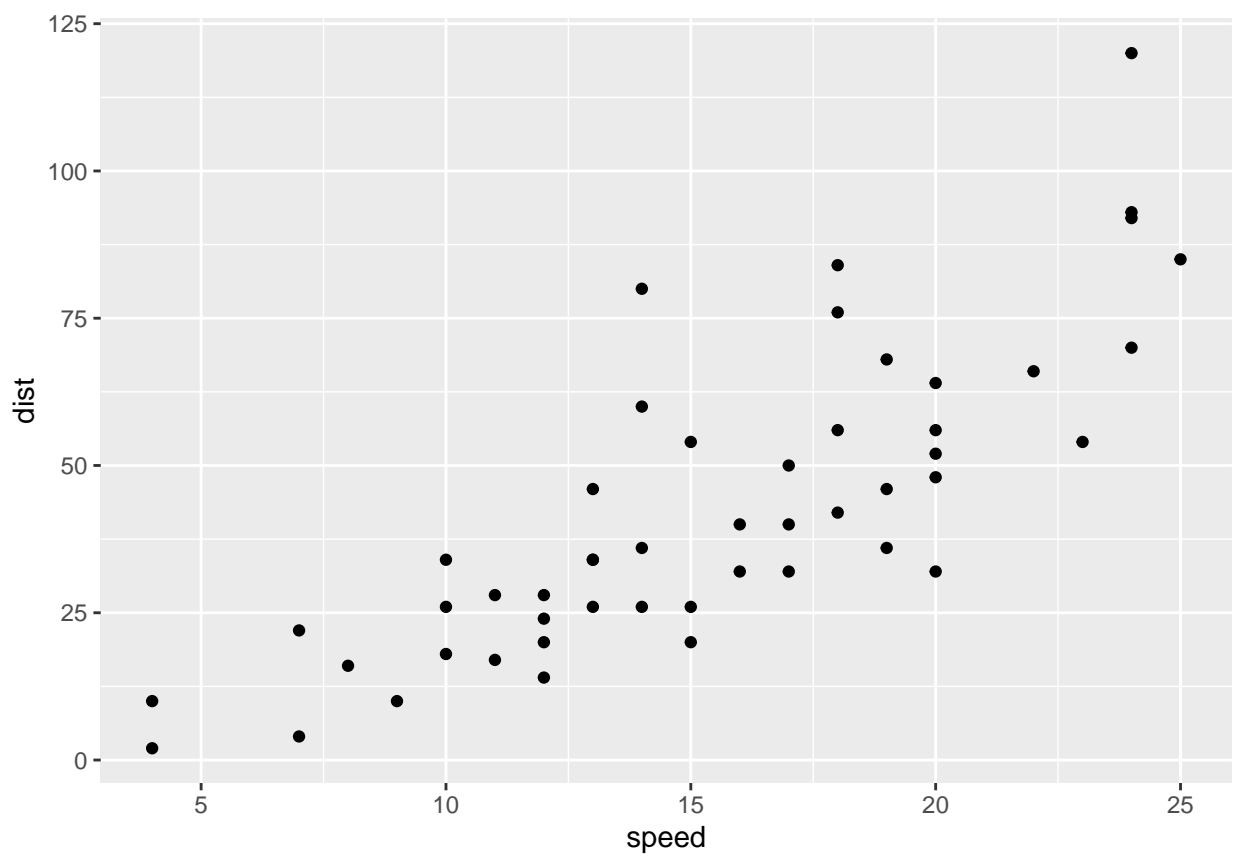


Figure 2.4: A ggplot of car stuff

Table 2.1: A knitr kable table

speed	dist
4	2
4	10
7	4
7	22
8	16
9	10

Under the hood, plots are included in your document in the same way as images - when you build the book or knit a chapter, the plot is automatically generated from your code, saved as an image, then included into the output document.

2.2.4 Including tables

Tables are usually included with the `kable` function from the `knitr` package.

Table 2.1 shows the first rows of that cars data - read in your own data, then use this approach to automatically generate tables.

```
cars %>%  
  head() %>%  
  knitr::kable(caption = "A knitr kable table")
```

- Gotcha: when using `kable`, captions are set inside the `kable` function
- The `kable` package is often used with the `kableExtra` package

2.2.5 Control positioning

One thing that may be annoying is the way *R Markdown* handles “floats” like tables and figures. In your PDF output, LaTeX will try to find the best place to put your object based on the text around it and until you’re really, truly done writing you should just leave it where it lies.

In general, you should allow LaTeX to do this, but if you really *really* need a figure to be positioned where you put in the document, then you can make LaTeX attempt to do this with the chunk option `fig.pos="H"`, as in Figure 2.5:

```
knitr::include_graphics("figures/sample-content/beltcrest.png")
```



Figure 2.5: An Oxford logo that LaTeX will try to place at this position in the text

As anyone who has tried to manually play around with the placement of figures in a Word document knows, this can have lots of side effects with extra spacing on other pages, etc. Therefore, it is not generally a good idea to do this - only do it when you really need to ensure that an image follows directly under text where you refer to it (in this document, I needed to do this for Figure 4.1 in section 4.1.4). For more details, read the relevant section of the [R Markdown Cookbook](#).

2.3 Executable inline code

‘Inline code’ simply means inclusion of code inside text. The syntax for doing this is ``r R_CODE``. For example, ``r 4 + 4`` will output 8 in your text.

You will usually use this in parts of your thesis where you report results - read in data or results in a code chunk, store things you want to report in a variable, then insert the value of that variable in your text. For example, we might assign the number of rows in the `cars` dataset to a variable:

2. *R Markdown basics*

```
num_car_observations <- nrow(cars)
```

We might then write:

“In the `cars` dataset, we have ``r num_car_observations`` observations.”

Which would output:

“In the `cars` dataset, we have 50 observations.”

2.4 Executable code in other languages than R

If you want to use other languages than R, such as Python, Julia C++, or SQL, see [the relevant section of the *R Markdown Cookbook*](#)

3

Citations, cross-references, and collaboration

Contents

3.1 Citations	24
3.1.1 PDF output	25
3.1.2 Gitbook output	26
3.1.3 Insert references easily with the <code>cittr</code> add-in	27
3.2 Cross-referencing	27
3.2.1 Section references	27
3.2.2 Figure (image and plot) references	28
3.2.3 Table references	28
3.2.4 Including page numbers	29
3.3 Collaborative writing	30
3.4 Additional resources	31

3.1 Citations

The usual way to include citations in an *R Markdown* document is to put references in a plain text file with the extension `.bib`, in **BibTeX** format.¹ Then reference the path to this file in `index.Rmd`'s YAML header with `bibliography: example.bib`.

¹The bibliography can be in other formats as well, including EndNote (`.enl`) and RIS (`.ris`), see rmarkdown.rstudio.com/authoring_bibliographies_and_citations.

3. Citations and cross-refs

Most reference managers can create a .bib file with your references automatically. However, the **by far** best reference manager to use with *R Markdown* is [Zotero](#) with the [Better BibTex plug-in](#), because the `citr` plugin for RStudio (see below) can read references directly from your Zotero library!

Here is an example of an entry in a .bib file:

```
@article{Shea2014,  
  author =      {Shea, Nicholas and Boldt, Annika},  
  journal =      {Trends in Cognitive Sciences},  
  pages =        {186--193},  
  title =        {{Supra-personal cognitive control}},  
  volume =       {18},  
  year =         {2014},  
  doi =          {10.1016/j.tics.2014.01.006},  
}
```

In this entry highlighted section, ‘Shea2014’ is the **citation identifier**. The default way to cite an entry in your text is with this syntax: `[@citation-identifier]`.

So I might cite some things [Shea2014, Lottridge2012].

3.1.1 PDF output

In PDF output, the bibliography is handled by the OxThesis LaTeX template. If you set `bib-humanities: true` in `index.Rmd`, then in-text references will be formatted as author-year; otherwise references will be shown as numbers.

If you choose author-year formatting, a number of variations on the citation syntax are useful to know:

- Put author names outside the parenthesis
 - This: `@Shea2014` says blah.
 - Becomes: **Shea2014** says blah.
- Include only the citation-year (in parenthesis)

3. Citations and cross-refs

- This: `Shea et al. says blah [-@Shea2014]`
- Becomes: `Shea et al. says blah [Shea2014]`
- Add text and page or chapter references to the citation
 - This: `[see @Shea2014, pp. 33-35; also @Wu2016, ch. 1]`
 - Becomes: `Blah blah [Shea2014, Wu2016].`

3.1.2 Gitbook output

In gitbook output, citations are by default inserted in the Chicago author-date format.

To change the format, add `csl: some-other-style.csl` in `index.Rmd`'s YAML header. You can browse through and download styles at zotero.org/styles.

3. Citations and cross-refs

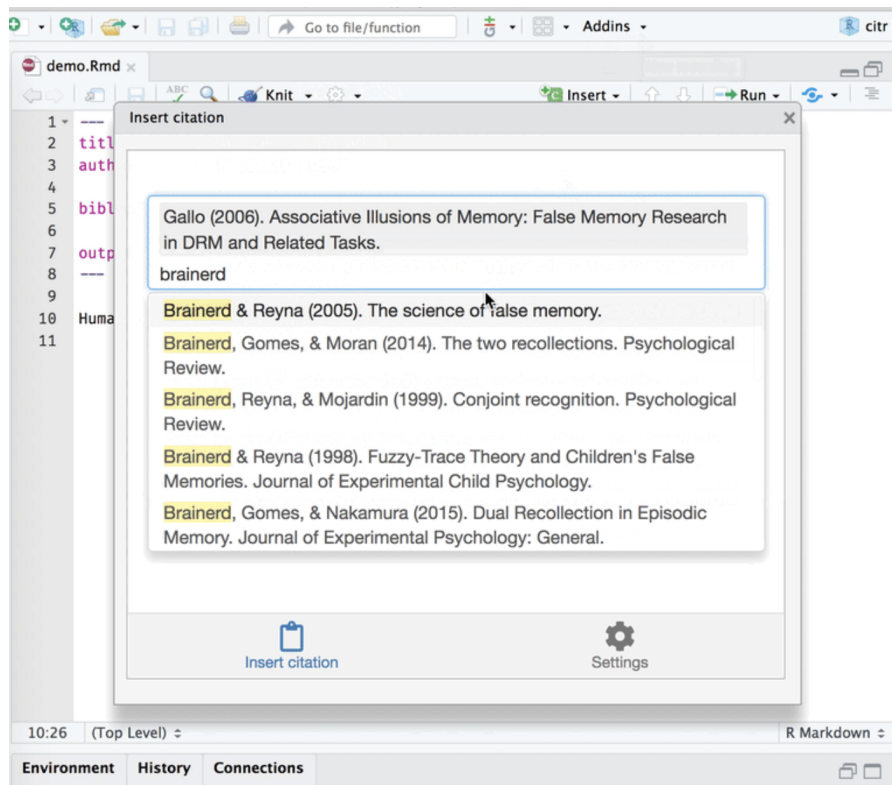


Figure 3.1: The ‘citr’ add-in

3.1.3 Insert references easily with the citr add-in

For an easy way to insert citations, try the `citr` RStudio add-in (Figure 3.1). You can install this add-in by typing `install.packages("citr")` in the R Console.

3.2 Cross-referencing

We can make cross-references to **sections** within our document, as well as to **figures** (images and plots) and **tables**.

The general cross-referencing syntax is `\@ref(label)`

3.2.1 Section references

Headers are automatically assigned a reference label, which is the text in lower caps separated by dashes. For example, `# My header` is automatically given the label `my-header`. So `# My header` can be referenced with `\@ref(my-section)`

3. Citations and cross-refs

Remember what we wrote in section 3.1?

We can also use **hyperlink syntax** and add # before the label, though this is only guaranteed to work properly in HTML output:

- So if we write Remember what we wrote up in [the previous section](#citations)?
- It becomes Remember what we wrote up in [the previous section](#)?

Creating custom labels

It is a very good idea to create **custom labels** for our sections. This is because the automatically assigned labels will change when we change the titles of the sections - to avoid this, we can create the labels ourselves and leave them untouched if we change the section titles.

We create custom labels by adding {#label} after a header, e.g. # My section {#my-label}. See [our chapter title](#) for an example. That was section 3.

3.2.2 Figure (image and plot) references

- To refer to figures (i.e. images and plots) use the syntax \@ref(fig:label)
- **GOTCHA:** Figures and tables must have captions if you wish to cross-reference them.

Let's add an image:

```
knitr::include_graphics("figures/sample-content/captain.jpeg")
```

We refer to this image with \@ref(fig:captain). So Figure 3.2 is [this image](#).

And in Figure 2.4 we saw a [cars plot](#).

3.2.3 Table references

- To refer to tables use the syntax \@ref(tab:label)

Let's include a table:

3. Citations and cross-refs



Figure 3.2: A marvel-lous meme

Table 3.1: Stopping cars

speed	dist
4	2
4	10
7	4
7	22
8	16

```
knitr::kable(cars[1:5,],  
             caption="Stopping cars")
```

We refer to this table with `\@ref(tab:cars-table2)`. So Table 3.1 is [this table](#). 3.1 magic reference

And in Table 2.1 we saw more or less [the same cars table](#).

3.2.4 Including page numbers

Finally, in the PDF output we might also want to include the page number of a reference, so that it's easy to find in physical printed output. LaTeX has a

3. Citations and cross-refs

command for this, which looks like this: `\pageref{fig/tab:label}` (note: curly braces, not parentheses)

When we output to PDF, we can use raw LaTeX directly in our .Rmd files. So if we wanted to include the page of the cars plot we could write:

- This: Figure `\@ref(fig:cars-plot)` on page `\pageref(fig:cars-plot)`
- Becomes: Figure 2.4 on page 20

Include page numbers only in PDF output

A problem here is that LaTeX commands don't display in HTML output, so in the gitbook output we'd see simply "Figure 2.4 on page".

One way to get around this is to use inline R code to insert the text, and use an `ifelse` statement to check the output format and then insert the appropriate text.

- So this: ``r ifelse(knitr::is_latex_output(), "Figure \@ref(fig:cars-plot) on page \pageref{fig:cars-plot}", "")``
- Inserts this (check this on both PDF and gitbook): Figure 2.4 on page 20

Note that we need to escape the backslash with another backslash here to get the correct output.

3.3 Collaborative writing

Best practices for collaboration and change tracking when using R Markdown are still an open question. In the blog post [One year to dissertate](#) by Lucy D'Agostino, which I highly recommend, the author notes that she knits .Rmd files to a word document, then uses the `googledrive` R package to send this to Google Drive for comments / revisions from co-authors, then incorporates Google Drive suggestions *by hand* into the .Rmd source files. This is a bit clunky, and there are ongoing discussions among the *R Markdown* developers about what the best way is to handle collaborative writing (see [issue #1463](#) on GitHub, where [CriticMarkup](#) is among the suggestions).

3. Citations and cross-refs

For now, this is an open question in the community of R Markdown users. I often knit to a format that can easily be imported to Google Docs for comments, then go over suggested revisions and manually incorporate them back in to the .Rmd source files. For articles, I sometimes upload a near-final draft to [Overleaf](#), then collaboratively make final edits to the LaTeX file there. I suspect some great solution will be developed in the not-to-distant future, probably by the RStudio team.

3.4 Additional resources

- *R Markdown: The Definitive Guide* - <https://bookdown.org/yihui/rmarkdown/>
- *R for Data Science* - <https://r4ds.had.co.nz>

4

Tables

Contents

4.1	Making LaTeX tables play nice	32
4.1.1	Making your table pretty	32
4.1.2	If your table is too wide	33
4.1.3	If your table is too long	34
4.1.4	Max power: manually adjust the raw LaTeX output . .	43

4.1 Making LaTeX tables play nice

Dealing with tables in LaTeX can be painful. This section explains the main tricks you need to make the pain go away.

(Note: if you are looking at the ebook version, you will not see much difference in this section, as it is only relevant for PDF output!)

4.1.1 Making your table pretty

When you use `kable` to create tables, you will almost certainly want to set the option `booktabs = TRUE`. This makes your table look a million times better:

4. Tables

```
library(knitr)
library(tidyverse)

head(mtcars) %>%
  kable(booktabs = TRUE)
```

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Mazda RX4	21.0	6	160	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag	21.0	6	160	110	3.90	2.875	17.02	0	1	4	4
Datsun 710	22.8	4	108	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive	21.4	6	258	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout	18.7	8	360	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225	105	2.76	3.460	20.22	1	0	3	1

Compare this to the default style, which looks terrible:

```
head(mtcars) %>%
  kable()
```

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Mazda RX4	21.0	6	160	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag	21.0	6	160	110	3.90	2.875	17.02	0	1	4	4
Datsun 710	22.8	4	108	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive	21.4	6	258	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout	18.7	8	360	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225	105	2.76	3.460	20.22	1	0	3	1

4.1.2 If your table is too wide

You might find that your table expands into the margins of the page, like the tables above. Fix this with the `kable_styling` function from the [kableExtra](#) package:

```
library(kableExtra)

head(mtcars) %>%
  kable(booktabs = TRUE) %>%
  kable_styling(latex_options = "scale_down")
```

This scales down the table to fit the page width.

4. Tables

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Mazda RX4	21.0	6	160	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag	21.0	6	160	110	3.90	2.875	17.02	0	1	4	4
Datsun 710	22.8	4	108	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive	21.4	6	258	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout	18.7	8	360	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225	105	2.76	3.460	20.22	1	0	3	1

4.1.3 If your table is too long

If your table is too long to fit on a single page, set `longtable = TRUE` in the `kable` function to split the table across multiple pages.

```
a_long_table <- rbind(mtcars, mtcars)

a_long_table %>%
  select(1:8) %>%
  kable(booktabs = TRUE, longtable = TRUE)
```

	mpg	cyl	disp	hp	drat	wt	qsec	vs
Mazda RX4	21.0	6	160.0	110	3.90	2.620	16.46	0
Mazda RX4 Wag	21.0	6	160.0	110	3.90	2.875	17.02	0
Datsun 710	22.8	4	108.0	93	3.85	2.320	18.61	1
Hornet 4 Drive	21.4	6	258.0	110	3.08	3.215	19.44	1
Hornet Sportabout	18.7	8	360.0	175	3.15	3.440	17.02	0
Valiant	18.1	6	225.0	105	2.76	3.460	20.22	1
Duster 360	14.3	8	360.0	245	3.21	3.570	15.84	0
Merc 240D	24.4	4	146.7	62	3.69	3.190	20.00	1
Merc 230	22.8	4	140.8	95	3.92	3.150	22.90	1
Merc 280	19.2	6	167.6	123	3.92	3.440	18.30	1
Merc 280C	17.8	6	167.6	123	3.92	3.440	18.90	1
Merc 450SE	16.4	8	275.8	180	3.07	4.070	17.40	0
Merc 450SL	17.3	8	275.8	180	3.07	3.730	17.60	0
Merc 450SLC	15.2	8	275.8	180	3.07	3.780	18.00	0
Cadillac Fleetwood	10.4	8	472.0	205	2.93	5.250	17.98	0
Lincoln Continental	10.4	8	460.0	215	3.00	5.424	17.82	0
Chrysler Imperial	14.7	8	440.0	230	3.23	5.345	17.42	0
Fiat 128	32.4	4	78.7	66	4.08	2.200	19.47	1
Honda Civic	30.4	4	75.7	52	4.93	1.615	18.52	1
Toyota Corolla	33.9	4	71.1	65	4.22	1.835	19.90	1

4. Tables

Toyota Corona	21.5	4	120.1	97	3.70	2.465	20.01	1
Dodge Challenger	15.5	8	318.0	150	2.76	3.520	16.87	0
AMC Javelin	15.2	8	304.0	150	3.15	3.435	17.30	0
Camaro Z28	13.3	8	350.0	245	3.73	3.840	15.41	0
Pontiac Firebird	19.2	8	400.0	175	3.08	3.845	17.05	0
Fiat X1-9	27.3	4	79.0	66	4.08	1.935	18.90	1
Porsche 914-2	26.0	4	120.3	91	4.43	2.140	16.70	0
Lotus Europa	30.4	4	95.1	113	3.77	1.513	16.90	1
Ford Pantera L	15.8	8	351.0	264	4.22	3.170	14.50	0
Ferrari Dino	19.7	6	145.0	175	3.62	2.770	15.50	0
Maserati Bora	15.0	8	301.0	335	3.54	3.570	14.60	0
Volvo 142E	21.4	4	121.0	109	4.11	2.780	18.60	1
Mazda RX41	21.0	6	160.0	110	3.90	2.620	16.46	0
Mazda RX4 Wag1	21.0	6	160.0	110	3.90	2.875	17.02	0
Datsun 7101	22.8	4	108.0	93	3.85	2.320	18.61	1
Hornet 4 Drive1	21.4	6	258.0	110	3.08	3.215	19.44	1
Hornet Sportabout1	18.7	8	360.0	175	3.15	3.440	17.02	0
Valiant1	18.1	6	225.0	105	2.76	3.460	20.22	1
Duster 3601	14.3	8	360.0	245	3.21	3.570	15.84	0
Merc 240D1	24.4	4	146.7	62	3.69	3.190	20.00	1
Merc 2301	22.8	4	140.8	95	3.92	3.150	22.90	1
Merc 2801	19.2	6	167.6	123	3.92	3.440	18.30	1
Merc 280C1	17.8	6	167.6	123	3.92	3.440	18.90	1
Merc 450SE1	16.4	8	275.8	180	3.07	4.070	17.40	0
Merc 450SL1	17.3	8	275.8	180	3.07	3.730	17.60	0
Merc 450SLC1	15.2	8	275.8	180	3.07	3.780	18.00	0
Cadillac Fleetwood1	10.4	8	472.0	205	2.93	5.250	17.98	0
Lincoln Continental1	10.4	8	460.0	215	3.00	5.424	17.82	0
Chrysler Imperial1	14.7	8	440.0	230	3.23	5.345	17.42	0
Fiat 1281	32.4	4	78.7	66	4.08	2.200	19.47	1
Honda Civic1	30.4	4	75.7	52	4.93	1.615	18.52	1
Toyota Corolla1	33.9	4	71.1	65	4.22	1.835	19.90	1
Toyota Corona1	21.5	4	120.1	97	3.70	2.465	20.01	1
Dodge Challenger1	15.5	8	318.0	150	2.76	3.520	16.87	0
AMC Javelin1	15.2	8	304.0	150	3.15	3.435	17.30	0
Camaro Z281	13.3	8	350.0	245	3.73	3.840	15.41	0
Pontiac Firebird1	19.2	8	400.0	175	3.08	3.845	17.05	0
Fiat X1-91	27.3	4	79.0	66	4.08	1.935	18.90	1
Porsche 914-21	26.0	4	120.3	91	4.43	2.140	16.70	0
Lotus Europa1	30.4	4	95.1	113	3.77	1.513	16.90	1
Ford Pantera L1	15.8	8	351.0	264	4.22	3.170	14.50	0
Ferrari Dino1	19.7	6	145.0	175	3.62	2.770	15.50	0

4. Tables

Maserati Bora	15.0	8	301.0	335	3.54	3.570	14.60	0
Volvo 142E	21.4	4	121.0	109	4.11	2.780	18.60	1

When you do this, you'll probably want to make the header repeat on new pages.

Do this with the `kable_styling` function from `kableExtra`:

```
a_long_table %>%
  kable(booktabs = TRUE, longtable = TRUE) %>%
  kable_styling(latex_options = "repeat_header")
```

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Mazda RX4	21.0	6	160.0	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag	21.0	6	160.0	110	3.90	2.875	17.02	0	1	4	4
Datsun 710	22.8	4	108.0	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive	21.4	6	258.0	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout	18.7	8	360.0	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225.0	105	2.76	3.460	20.22	1	0	3	1
Duster 360	14.3	8	360.0	245	3.21	3.570	15.84	0	0	3	4
Merc 240D	24.4	4	146.7	62	3.69	3.190	20.00	1	0	4	2
Merc 230	22.8	4	140.8	95	3.92	3.150	22.90	1	0	4	2
Merc 280	19.2	6	167.6	123	3.92	3.440	18.30	1	0	4	4
Merc 280C	17.8	6	167.6	123	3.92	3.440	18.90	1	0	4	4
Merc 450SE	16.4	8	275.8	180	3.07	4.070	17.40	0	0	3	3
Merc 450SL	17.3	8	275.8	180	3.07	3.730	17.60	0	0	3	3
Merc 450SLC	15.2	8	275.8	180	3.07	3.780	18.00	0	0	3	3
Cadillac Fleetwood	10.4	8	472.0	205	2.93	5.250	17.98	0	0	3	4
Lincoln Continental	10.4	8	460.0	215	3.00	5.424	17.82	0	0	3	4
Chrysler Imperial	14.7	8	440.0	230	3.23	5.345	17.42	0	0	3	4
Fiat 128	32.4	4	78.7	66	4.08	2.200	19.47	1	1	4	1
Honda Civic	30.4	4	75.7	52	4.93	1.615	18.52	1	1	4	2
Toyota Corolla	33.9	4	71.1	65	4.22	1.835	19.90	1	1	4	1
Toyota Corona	21.5	4	120.1	97	3.70	2.465	20.01	1	0	3	1
Dodge Challenger	15.5	8	318.0	150	2.76	3.520	16.87	0	0	3	2
AMC Javelin	15.2	8	304.0	150	3.15	3.435	17.30	0	0	3	2
Camaro Z28	13.3	8	350.0	245	3.73	3.840	15.41	0	0	3	4
Pontiac Firebird	19.2	8	400.0	175	3.08	3.845	17.05	0	0	3	2
Fiat X1-9	27.3	4	79.0	66	4.08	1.935	18.90	1	1	4	1
Porsche 914-2	26.0	4	120.3	91	4.43	2.140	16.70	0	1	5	2
Lotus Europa	30.4	4	95.1	113	3.77	1.513	16.90	1	1	5	2
Ford Pantera L	15.8	8	351.0	264	4.22	3.170	14.50	0	1	5	4
Ferrari Dino	19.7	6	145.0	175	3.62	2.770	15.50	0	1	5	6

4. Tables

(continued)

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Maserati Bora	15.0	8	301.0	335	3.54	3.570	14.60	0	1	5	8
Volvo 142E	21.4	4	121.0	109	4.11	2.780	18.60	1	1	4	2
Mazda RX41	21.0	6	160.0	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag1	21.0	6	160.0	110	3.90	2.875	17.02	0	1	4	4
Datsun 7101	22.8	4	108.0	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive1	21.4	6	258.0	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout1	18.7	8	360.0	175	3.15	3.440	17.02	0	0	3	2
Valiant1	18.1	6	225.0	105	2.76	3.460	20.22	1	0	3	1
Duster 3601	14.3	8	360.0	245	3.21	3.570	15.84	0	0	3	4
Merc 240D1	24.4	4	146.7	62	3.69	3.190	20.00	1	0	4	2
Merc 2301	22.8	4	140.8	95	3.92	3.150	22.90	1	0	4	2
Merc 2801	19.2	6	167.6	123	3.92	3.440	18.30	1	0	4	4
Merc 280C1	17.8	6	167.6	123	3.92	3.440	18.90	1	0	4	4
Merc 450SE1	16.4	8	275.8	180	3.07	4.070	17.40	0	0	3	3
Merc 450SL1	17.3	8	275.8	180	3.07	3.730	17.60	0	0	3	3
Merc 450SLC1	15.2	8	275.8	180	3.07	3.780	18.00	0	0	3	3
Cadillac Fleetwood1	10.4	8	472.0	205	2.93	5.250	17.98	0	0	3	4
Lincoln Continental1	10.4	8	460.0	215	3.00	5.424	17.82	0	0	3	4
Chrysler Imperial1	14.7	8	440.0	230	3.23	5.345	17.42	0	0	3	4
Fiat 1281	32.4	4	78.7	66	4.08	2.200	19.47	1	1	4	1
Honda Civic1	30.4	4	75.7	52	4.93	1.615	18.52	1	1	4	2
Toyota Corolla1	33.9	4	71.1	65	4.22	1.835	19.90	1	1	4	1
Toyota Corona1	21.5	4	120.1	97	3.70	2.465	20.01	1	0	3	1
Dodge Challenger1	15.5	8	318.0	150	2.76	3.520	16.87	0	0	3	2
AMC Javelin1	15.2	8	304.0	150	3.15	3.435	17.30	0	0	3	2
Camaro Z281	13.3	8	350.0	245	3.73	3.840	15.41	0	0	3	4
Pontiac Firebird1	19.2	8	400.0	175	3.08	3.845	17.05	0	0	3	2
Fiat X1-91	27.3	4	79.0	66	4.08	1.935	18.90	1	1	4	1
Porsche 914-21	26.0	4	120.3	91	4.43	2.140	16.70	0	1	5	2
Lotus Europa1	30.4	4	95.1	113	3.77	1.513	16.90	1	1	5	2
Ford Pantera L1	15.8	8	351.0	264	4.22	3.170	14.50	0	1	5	4
Ferrari Dino1	19.7	6	145.0	175	3.62	2.770	15.50	0	1	5	6
Maserati Bora1	15.0	8	301.0	335	3.54	3.570	14.60	0	1	5	8
Volvo 142E1	21.4	4	121.0	109	4.11	2.780	18.60	1	1	4	2

Unfortunately, we cannot use the `scale_down` option with a `longtable`. So if a `longtable` is too wide, you can either manually adjust the font size, or show the table in landscape layout. To adjust the font size, use `kableExtra`'s `font_size` option:

4. Tables

```
a_long_table %>%
```

```
  kable(booktabs = TRUE, longtable = TRUE) %>%
```

```
  kable_styling(font_size = 9, latex_options = "repeat_header")
```

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Mazda RX4	21.0	6	160.0	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag	21.0	6	160.0	110	3.90	2.875	17.02	0	1	4	4
Datsun 710	22.8	4	108.0	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive	21.4	6	258.0	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout	18.7	8	360.0	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225.0	105	2.76	3.460	20.22	1	0	3	1
Duster 360	14.3	8	360.0	245	3.21	3.570	15.84	0	0	3	4
Merc 240D	24.4	4	146.7	62	3.69	3.190	20.00	1	0	4	2
Merc 230	22.8	4	140.8	95	3.92	3.150	22.90	1	0	4	2
Merc 280	19.2	6	167.6	123	3.92	3.440	18.30	1	0	4	4
Merc 280C	17.8	6	167.6	123	3.92	3.440	18.90	1	0	4	4
Merc 450SE	16.4	8	275.8	180	3.07	4.070	17.40	0	0	3	3
Merc 450SL	17.3	8	275.8	180	3.07	3.730	17.60	0	0	3	3
Merc 450SLC	15.2	8	275.8	180	3.07	3.780	18.00	0	0	3	3
Cadillac Fleetwood	10.4	8	472.0	205	2.93	5.250	17.98	0	0	3	4
Lincoln Continental	10.4	8	460.0	215	3.00	5.424	17.82	0	0	3	4
Chrysler Imperial	14.7	8	440.0	230	3.23	5.345	17.42	0	0	3	4
Fiat 128	32.4	4	78.7	66	4.08	2.200	19.47	1	1	4	1
Honda Civic	30.4	4	75.7	52	4.93	1.615	18.52	1	1	4	2
Toyota Corolla	33.9	4	71.1	65	4.22	1.835	19.90	1	1	4	1
Toyota Corona	21.5	4	120.1	97	3.70	2.465	20.01	1	0	3	1
Dodge Challenger	15.5	8	318.0	150	2.76	3.520	16.87	0	0	3	2
AMC Javelin	15.2	8	304.0	150	3.15	3.435	17.30	0	0	3	2
Camaro Z28	13.3	8	350.0	245	3.73	3.840	15.41	0	0	3	4
Pontiac Firebird	19.2	8	400.0	175	3.08	3.845	17.05	0	0	3	2
Fiat X1-9	27.3	4	79.0	66	4.08	1.935	18.90	1	1	4	1
Porsche 914-2	26.0	4	120.3	91	4.43	2.140	16.70	0	1	5	2
Lotus Europa	30.4	4	95.1	113	3.77	1.513	16.90	1	1	5	2
Ford Pantera L	15.8	8	351.0	264	4.22	3.170	14.50	0	1	5	4
Ferrari Dino	19.7	6	145.0	175	3.62	2.770	15.50	0	1	5	6
Maserati Bora	15.0	8	301.0	335	3.54	3.570	14.60	0	1	5	8
Volvo 142E	21.4	4	121.0	109	4.11	2.780	18.60	1	1	4	2
Mazda RX41	21.0	6	160.0	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag1	21.0	6	160.0	110	3.90	2.875	17.02	0	1	4	4
Datsun 7101	22.8	4	108.0	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive1	21.4	6	258.0	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout1	18.7	8	360.0	175	3.15	3.440	17.02	0	0	3	2
Valiant1	18.1	6	225.0	105	2.76	3.460	20.22	1	0	3	1
Duster 3601	14.3	8	360.0	245	3.21	3.570	15.84	0	0	3	4
Merc 240D1	24.4	4	146.7	62	3.69	3.190	20.00	1	0	4	2
Merc 2301	22.8	4	140.8	95	3.92	3.150	22.90	1	0	4	2
Merc 2801	19.2	6	167.6	123	3.92	3.440	18.30	1	0	4	4
Merc 280C1	17.8	6	167.6	123	3.92	3.440	18.90	1	0	4	4
Merc 450SE1	16.4	8	275.8	180	3.07	4.070	17.40	0	0	3	3
Merc 450SL1	17.3	8	275.8	180	3.07	3.730	17.60	0	0	3	3
Merc 450SLC1	15.2	8	275.8	180	3.07	3.780	18.00	0	0	3	3
Cadillac Fleetwood1	10.4	8	472.0	205	2.93	5.250	17.98	0	0	3	4

4. Tables

(continued)

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Lincoln Continental1	10.4	8	460.0	215	3.00	5.424	17.82	0	0	3	4
Chrysler Imperial1	14.7	8	440.0	230	3.23	5.345	17.42	0	0	3	4
Fiat 1281	32.4	4	78.7	66	4.08	2.200	19.47	1	1	4	1
Honda Civic1	30.4	4	75.7	52	4.93	1.615	18.52	1	1	4	2
Toyota Corolla1	33.9	4	71.1	65	4.22	1.835	19.90	1	1	4	1
Toyota Corona1	21.5	4	120.1	97	3.70	2.465	20.01	1	0	3	1
Dodge Challenger1	15.5	8	318.0	150	2.76	3.520	16.87	0	0	3	2
AMC Javelin1	15.2	8	304.0	150	3.15	3.435	17.30	0	0	3	2
Camaro Z281	13.3	8	350.0	245	3.73	3.840	15.41	0	0	3	4
Pontiac Firebird1	19.2	8	400.0	175	3.08	3.845	17.05	0	0	3	2
Fiat X1-91	27.3	4	79.0	66	4.08	1.935	18.90	1	1	4	1
Porsche 914-21	26.0	4	120.3	91	4.43	2.140	16.70	0	1	5	2
Lotus Europa1	30.4	4	95.1	113	3.77	1.513	16.90	1	1	5	2
Ford Pantera L1	15.8	8	351.0	264	4.22	3.170	14.50	0	1	5	4
Ferrari Dino1	19.7	6	145.0	175	3.62	2.770	15.50	0	1	5	6
Maserati Bora1	15.0	8	301.0	335	3.54	3.570	14.60	0	1	5	8
Volvo 142E1	21.4	4	121.0	109	4.11	2.780	18.60	1	1	4	2

To put the table in landscape mode, use kableExtra's `landscape` function:

```
a_long_table %>%
  kable(booktabs = TRUE, longtable = TRUE) %>%
  kable_styling(latex_options = "repeat_header") %>%
  landscape()
```


	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Mazda RX4	21.0	6	160.0	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag	21.0	6	160.0	110	3.90	2.875	17.02	0	1	4	4
Datsun 710	22.8	4	108.0	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive	21.4	6	258.0	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout	18.7	8	360.0	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225.0	105	2.76	3.460	20.22	1	0	3	1
Duster 360	14.3	8	360.0	245	3.21	3.570	15.84	0	0	3	4
Merc 240D	24.4	4	146.7	62	3.69	3.190	20.00	1	0	4	2
Merc 230	22.8	4	140.8	95	3.92	3.150	22.90	1	0	4	2
Merc 280	19.2	6	167.6	123	3.92	3.440	18.30	1	0	4	4
Merc 280C	17.8	6	167.6	123	3.92	3.440	18.90	1	0	4	4
Merc 450SE	16.4	8	275.8	180	3.07	4.070	17.40	0	0	3	3
Merc 450SL	17.3	8	275.8	180	3.07	3.730	17.60	0	0	3	3
Merc 450SLC	15.2	8	275.8	180	3.07	3.780	18.00	0	0	3	3
Cadillac Fleetwood	10.4	8	472.0	205	2.93	5.250	17.98	0	0	3	4
Lincoln Continental	10.4	8	460.0	215	3.00	5.424	17.82	0	0	3	4
Chrysler Imperial	14.7	8	440.0	230	3.23	5.345	17.42	0	0	3	4
Fiat 128	32.4	4	78.7	66	4.08	2.200	19.47	1	1	4	1
Honda Civic	30.4	4	75.7	52	4.93	1.615	18.52	1	1	4	2
Toyota Corolla	33.9	4	71.1	65	4.22	1.835	19.90	1	1	4	1
Toyota Corona	21.5	4	120.1	97	3.70	2.465	20.01	1	0	3	1
Dodge Challenger	15.5	8	318.0	150	2.76	3.520	16.87	0	0	3	2
AMC Javelin	15.2	8	304.0	150	3.15	3.435	17.30	0	0	3	2
Camaro Z28	13.3	8	350.0	245	3.73	3.840	15.41	0	0	3	4
Pontiac Firebird	19.2	8	400.0	175	3.08	3.845	17.05	0	0	3	2

(continued)

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Fiat X1-9	27.3	4	79.0	66	4.08	1.935	18.90	1	1	4	1
Porsche 914-2	26.0	4	120.3	91	4.43	2.140	16.70	0	1	5	2
Lotus Europa	30.4	4	95.1	113	3.77	1.513	16.90	1	1	5	2
Ford Pantera L	15.8	8	351.0	264	4.22	3.170	14.50	0	1	5	4
Ferrari Dino	19.7	6	145.0	175	3.62	2.770	15.50	0	1	5	6
Maserati Bora	15.0	8	301.0	335	3.54	3.570	14.60	0	1	5	8
Volvo 142E	21.4	4	121.0	109	4.11	2.780	18.60	1	1	4	2
Mazda RX41	21.0	6	160.0	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag1	21.0	6	160.0	110	3.90	2.875	17.02	0	1	4	4
Datsun 7101	22.8	4	108.0	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive1	21.4	6	258.0	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout1	18.7	8	360.0	175	3.15	3.440	17.02	0	0	3	2
Valiant1	18.1	6	225.0	105	2.76	3.460	20.22	1	0	3	1
Duster 3601	14.3	8	360.0	245	3.21	3.570	15.84	0	0	3	4
Merc 240D1	24.4	4	146.7	62	3.69	3.190	20.00	1	0	4	2
Merc 2301	22.8	4	140.8	95	3.92	3.150	22.90	1	0	4	2
Merc 2801	19.2	6	167.6	123	3.92	3.440	18.30	1	0	4	4
Merc 280C1	17.8	6	167.6	123	3.92	3.440	18.90	1	0	4	4
Merc 450SE1	16.4	8	275.8	180	3.07	4.070	17.40	0	0	3	3
Merc 450SL1	17.3	8	275.8	180	3.07	3.730	17.60	0	0	3	3
Merc 450SLC1	15.2	8	275.8	180	3.07	3.780	18.00	0	0	3	3
Cadillac Fleetwood1	10.4	8	472.0	205	2.93	5.250	17.98	0	0	3	4
Lincoln Continental1	10.4	8	460.0	215	3.00	5.424	17.82	0	0	3	4
Chrysler Imperial1	14.7	8	440.0	230	3.23	5.345	17.42	0	0	3	4

(continued)

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Fiat 1281	32.4	4	78.7	66	4.08	2.200	19.47	1	1	4	1
Honda Civic1	30.4	4	75.7	52	4.93	1.615	18.52	1	1	4	2
Toyota Corolla1	33.9	4	71.1	65	4.22	1.835	19.90	1	1	4	1
Toyota Corona1	21.5	4	120.1	97	3.70	2.465	20.01	1	0	3	1
Dodge Challenger1	15.5	8	318.0	150	2.76	3.520	16.87	0	0	3	2
AMC Javelin1	15.2	8	304.0	150	3.15	3.435	17.30	0	0	3	2
Camaro Z281	13.3	8	350.0	245	3.73	3.840	15.41	0	0	3	4
Pontiac Firebird1	19.2	8	400.0	175	3.08	3.845	17.05	0	0	3	2
Fiat X1-91	27.3	4	79.0	66	4.08	1.935	18.90	1	1	4	1
Porsche 914-21	26.0	4	120.3	91	4.43	2.140	16.70	0	1	5	2
Lotus Europa1	30.4	4	95.1	113	3.77	1.513	16.90	1	1	5	2
Ford Pantera L1	15.8	8	351.0	264	4.22	3.170	14.50	0	1	5	4
Ferrari Dino1	19.7	6	145.0	175	3.62	2.770	15.50	0	1	5	6
Maserati Bora1	15.0	8	301.0	335	3.54	3.570	14.60	0	1	5	8
Volvo 142E1	21.4	4	121.0	109	4.11	2.780	18.60	1	1	4	2

4.1.4 Max power: manually adjust the raw LaTeX output

For total flexibility, you can adjust the raw LaTeX output from `kable/kableExtra` that generates the table. Let us consider how we would do this for the example of adjusting the font size if our table is too wide: Latex has a bunch of standard commands that set an approximate font size, as shown below in Figure 4.1.

<code>\tiny</code>	Lorem ipsum
<code>\scriptsize</code>	Lorem ipsum
<code>\footnotesize</code>	Lorem ipsum
<code>\small</code>	Lorem ipsum

Figure 4.1: Font sizes in LaTeX

You could use these to manually adjust the font size in your longtable in two steps:

1. Wrap the longtable environment in, e.g., a `scriptsize` environment, by doing a string replacement in the output from `kable/kableExtra`
2. Add the attributes that make R Markdown understand that the table is a table (it seems R drops these when we do the string replacement)

```
our_adjusted_table <- a_long_table %>%
  kable(booktabs = TRUE, longtable = TRUE) %>%
  kable_styling(latex_options = "repeat_header") %>%
  # wrap the longtable in a tiny environment
  str_replace('\\\\begin\\{longtable\\}',
              '\\\\begin\\{scriptsize\\}\\n\\\\begin\\{longtable\\}') %>%
  str_replace('\\\\end\\{longtable\\}',
              '\\\\end\\{longtable\\}\\n\\\\end\\{scriptsize\\}')
```

4. Tables

#add attributes to make R Markdown treat this as a kable LaTeX table again

```
our_adjusted_table %>%
```

```
  structure(format = "latex", class = "knitr_kable")
```

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Mazda RX4	21.0	6	160.0	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag	21.0	6	160.0	110	3.90	2.875	17.02	0	1	4	4
Datsun 710	22.8	4	108.0	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive	21.4	6	258.0	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout	18.7	8	360.0	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225.0	105	2.76	3.460	20.22	1	0	3	1
Duster 360	14.3	8	360.0	245	3.21	3.570	15.84	0	0	3	4
Merc 240D	24.4	4	146.7	62	3.69	3.190	20.00	1	0	4	2
Merc 230	22.8	4	140.8	95	3.92	3.150	22.90	1	0	4	2
Merc 280	19.2	6	167.6	123	3.92	3.440	18.30	1	0	4	4
Merc 280C	17.8	6	167.6	123	3.92	3.440	18.90	1	0	4	4
Merc 450SE	16.4	8	275.8	180	3.07	4.070	17.40	0	0	3	3
Merc 450SL	17.3	8	275.8	180	3.07	3.730	17.60	0	0	3	3
Merc 450SLC	15.2	8	275.8	180	3.07	3.780	18.00	0	0	3	3
Cadillac Fleetwood	10.4	8	472.0	205	2.93	5.250	17.98	0	0	3	4
Lincoln Continental	10.4	8	460.0	215	3.00	5.424	17.82	0	0	3	4
Chrysler Imperial	14.7	8	440.0	230	3.23	5.345	17.42	0	0	3	4
Fiat 128	32.4	4	78.7	66	4.08	2.200	19.47	1	1	4	1
Honda Civic	30.4	4	75.7	52	4.93	1.615	18.52	1	1	4	2
Toyota Corolla	33.9	4	71.1	65	4.22	1.835	19.90	1	1	4	1
Toyota Corona	21.5	4	120.1	97	3.70	2.465	20.01	1	0	3	1
Dodge Challenger	15.5	8	318.0	150	2.76	3.520	16.87	0	0	3	2
AMC Javelin	15.2	8	304.0	150	3.15	3.435	17.30	0	0	3	2
Camaro Z28	13.3	8	350.0	245	3.73	3.840	15.41	0	0	3	4
Pontiac Firebird	19.2	8	400.0	175	3.08	3.845	17.05	0	0	3	2
Fiat X1-9	27.3	4	79.0	66	4.08	1.935	18.90	1	1	4	1
Porsche 914-2	26.0	4	120.3	91	4.43	2.140	16.70	0	1	5	2
Lotus Europa	30.4	4	95.1	113	3.77	1.513	16.90	1	1	5	2
Ford Pantera L	15.8	8	351.0	264	4.22	3.170	14.50	0	1	5	4
Ferrari Dino	19.7	6	145.0	175	3.62	2.770	15.50	0	1	5	6
Maserati Bora	15.0	8	301.0	335	3.54	3.570	14.60	0	1	5	8
Volvo 142E	21.4	4	121.0	109	4.11	2.780	18.60	1	1	4	2
Mazda RX41	21.0	6	160.0	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag1	21.0	6	160.0	110	3.90	2.875	17.02	0	1	4	4
Datsun 7101	22.8	4	108.0	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive1	21.4	6	258.0	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout1	18.7	8	360.0	175	3.15	3.440	17.02	0	0	3	2
Valiant1	18.1	6	225.0	105	2.76	3.460	20.22	1	0	3	1
Duster 3601	14.3	8	360.0	245	3.21	3.570	15.84	0	0	3	4
Merc 240D1	24.4	4	146.7	62	3.69	3.190	20.00	1	0	4	2
Merc 2301	22.8	4	140.8	95	3.92	3.150	22.90	1	0	4	2
Merc 2801	19.2	6	167.6	123	3.92	3.440	18.30	1	0	4	4
Merc 280C1	17.8	6	167.6	123	3.92	3.440	18.90	1	0	4	4
Merc 450SE1	16.4	8	275.8	180	3.07	4.070	17.40	0	0	3	3
Merc 450SL1	17.3	8	275.8	180	3.07	3.730	17.60	0	0	3	3
Merc 450SLC1	15.2	8	275.8	180	3.07	3.780	18.00	0	0	3	3
Cadillac Fleetwood1	10.4	8	472.0	205	2.93	5.250	17.98	0	0	3	4
Lincoln Continental1	10.4	8	460.0	215	3.00	5.424	17.82	0	0	3	4
Chrysler Imperial1	14.7	8	440.0	230	3.23	5.345	17.42	0	0	3	4
Fiat 1281	32.4	4	78.7	66	4.08	2.200	19.47	1	1	4	1
Honda Civic1	30.4	4	75.7	52	4.93	1.615	18.52	1	1	4	2
Toyota Corolla1	33.9	4	71.1	65	4.22	1.835	19.90	1	1	4	1

4. Tables

(continued)

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Toyota Corona1	21.5	4	120.1	97	3.70	2.465	20.01	1	0	3	1
Dodge Challenger1	15.5	8	318.0	150	2.76	3.520	16.87	0	0	3	2
AMC Javelin1	15.2	8	304.0	150	3.15	3.435	17.30	0	0	3	2
Camaro Z281	13.3	8	350.0	245	3.73	3.840	15.41	0	0	3	4
Pontiac Firebird1	19.2	8	400.0	175	3.08	3.845	17.05	0	0	3	2
Fiat X1-91	27.3	4	79.0	66	4.08	1.935	18.90	1	1	4	1
Porsche 914-21	26.0	4	120.3	91	4.43	2.140	16.70	0	1	5	2
Lotus Europa1	30.4	4	95.1	113	3.77	1.513	16.90	1	1	5	2
Ford Pantera L1	15.8	8	351.0	264	4.22	3.170	14.50	0	1	5	4
Ferrari Dino1	19.7	6	145.0	175	3.62	2.770	15.50	0	1	5	6
Maserati Bora1	15.0	8	301.0	335	3.54	3.570	14.60	0	1	5	8
Volvo 142E1	21.4	4	121.0	109	4.11	2.780	18.60	1	1	4	2

There is grandeur in this view of life, with its several powers, having been originally breathed into a few forms or into one; and that, whilst this planet has gone cycling on according to the fixed law of gravity, from so simple a beginning endless forms most beautiful and most wonderful have been, and are being, evolved.

— Charles Darwin [Darwin1859]

5

Customisations and extensions

Contents

5.1	Front matter	47
5.1.1	Shorten captions shown in the list of figures (PDF)	47
5.1.2	Shorten captions shown in the list of tables (PDF)	47
5.2	Shorten running header (PDF)	48
5.3	Unnumbered chapters	48
5.4	Beginning chapters with quotes (PDF)	48
5.5	Highlighting corrections (HTML & PDF)	49
5.5.1	Short, inline corrections	49
5.5.2	Blocks of added or changed material	50
5.5.3	Stopping corrections from being highlighted	50
5.6	Apply custom font color and highlighting to text (HTML & PDF)	50
5.7	Including another paper in your thesis - embed a PDF document	51
5.8	Including another paper in your thesis - R Markdown child document	55
5.8.1	An example paper in another folder	55
5.8.2	Step 1: Include paper as a child document	56
5.8.3	Step 2: Make file paths compatible	56
5.8.4	Step 3: Make sure header levels are correct	57
5.8.5	Step 4: Make sure figure widths are correct	58
5.9	Customizing referencing	59
5.9.1	Using a .csl file with pandoc instead of biblatex	59
5.9.2	Customizing biblatex and adding chapter bibliographies	59
5.10	Customizing the page headers and footers (PDF)	62
5.11	Diving in to the OxThesis LaTeX template (PDF)	63
5.12	Customising to a different university	63
5.12.1	The minimal route	63

This chapter describes a number of additional tips and tricks as well as possible customizations to the `oxforddown` thesis.

5.1 Front matter

5.1.1 Shorten captions shown in the list of figures (PDF)

You might want your list of figures (which follows the table of contents) to have shorter (or just different) figure descriptions than the actual figure captions.

Do this using the chunk option `fig.scap` ('short caption'), for example `{r captain-image, fig.cap="A very long and descriptive (and potentially boring) caption that doesn't fit in the list of figures, but helps the reader understand what the figure communicates.", fig.scap="A concise description for the list of figures"`

5.1.2 Shorten captions shown in the list of tables (PDF)

You might want your list of tables (which follows the list of figures in your thesis front matter) to have shorter (or just different) table descriptions than the actual table captions.

If you are using `knitr::kable` to generate a table, you can do this with the argument `caption.short`, e.g.:

```
knitr::kable(mtcars,
             caption = "A very long and descriptive (and potentially
             boring) caption that doesn't fit in the list of figures,
             but helps the reader understand what the figure
             communicates.",
             caption.short = "A concise description for the list of tables")
```


5.2 Shorten running header (PDF)

You might want a chapter's running header (i.e. the header showing the title of the current chapter at the top of page) to be shorter (or just different) to the actual chapter title.

Do this by adding the latex command `\chaptermark{My shorter version}` after your chapter title.

For example, chapter 3's running header is simply 'Cites and cross-refs', because it begins like this:

```
# Citations, cross-references, and collaboration {#cites-and-refs}
\chaptermark{Cites and cross-refs}
```

5.3 Unnumbered chapters

To make chapters unnumbered (normally only relevant to the Introduction and/or the Conclusion), follow the chapter header with `{-}`, e.g. `# Introduction {-}`.

When you do this, you must also follow the heading with these two latex commands:

```
\adjustmtc
\markboth{The Name of Your Unnumbered Chapter}{{}}
```

Otherwise the chapter's mini table of contents and the running header will show the previous chapter.

5.4 Beginning chapters with quotes (PDF)

The OxThesis LaTeX template lets you inject some wittiness into your thesis by including a block of type `savequote` at the beginning of chapters. To do this, use the syntax ````\block type='savequote'}`.¹

¹For more on custom block types, see the relevant section in *Authoring Books with R Markdown*.

5. Customisations and extensions

Add the reference for the quote with the chunk option `quote_author="my author name"`. You will also want to add the chunk option `include=knitr::is_latex_output()` so that quotes are only included in PDF output.

It's not possible to use markdown syntax inside chunk options, so if you want to e.g. italicise a book name in the reference use a `'text reference'`: Create a named piece of text with `'(ref:label-name) My text'`, then point to this in the chunk option with `quote_author='(ref:label-name)'`.

5.5 Highlighting corrections (HTML & PDF)

For when it comes time to do corrections, you may want to highlight changes made when you submit a post-viva, corrected copy to your examiners so they can quickly verify you've completed the task. You can do so like this:

5.5.1 Short, inline corrections

Highlight **short, inline corrections** by doing `[like this]{.correction}` — the text between the square brackets will then be highlighted in blue in the output.

Note that pandoc might get confused by citations and cross-references inside inline corrections. In particular, it might get confused by `"[what @Shea2014 said]{.correction}"` which becomes `[Shea2014]{.correction}` In such cases, you can use LaTeX syntax directly. The correction highlighting uses the `soul` package, so you can do like this:

- If using biblatex for references, use `"\hl{what \textcite{Shea2014} said}"`
- If using natbib for references, use `"\hl{what \cite{Shea2014} said}"`

Using raw LaTeX has the drawback of corrections then not showing up in HTML output at all, but you might only care about correction highlighting in the PDF for your examiners anyway!

5. Customisations and extensions

5.5.2 Blocks of added or changed material

Highlight entire **blocks of added or changed material** by putting them in a block of type `correction`, using the syntax ````{block type='correction'}````.² Like so:

For larger chunks, like this paragraph or indeed entire figures, you can use the `correction` block type. This environment **highlights paragraph-sized and larger blocks** with the same blue colour.

Note that correction blocks cannot be included in word output.

5.5.3 Stopping corrections from being highlighted

To turn off correction highlighting, go to the YAML header of `index.Rmd`, then:

- PDF output: set `corrections: false`
- HTML output: remove or comment out - `templates/corrections.css`

5.6 Apply custom font color and highlighting to text (HTML & PDF)

The lua filter that adds the functionality to highlight corrections adds two more tricks: you can apply your own choice of colour to highlight text, or change the font color. The syntax is as follows:

Here's `[some text in pink highlighting]{highlight="pink"}`
Becomes: Here's `some text in pink highlighting`.

`[Here's some text with blue font]{color="blue"}`
Becomes: `Here's some text with blue font`

Finally — never, ever actually do this — `[here's some text with black highlighting and yellow font]{highlight="black" color="yellow"}`
Becomes: `here's some text with black highlighting and yellow font`

²In the `.tex` file for PDF output, this will put the content between `\begin{correction}` and `\end{correction}`; in gitbook output it will be put between `<div class="correction">` and `</div>`.

5. Customisations and extensions

The file `scripts__and__filters/colour__and__highlight.lua` implements this, if you want to fiddle around with it. It works with both PDF and HTML output.

5.7 Including another paper in your thesis - embed a PDF document

You may want to embed existing PDF documents into the thesis, for example if your department allows a ‘portfolio’ style thesis and you need to include an existing typeset publication as a chapter.

In gitbook output, you can simply use `knitr::include_graphics` and it should include a scrollable (and downloadable) PDF. You will probably want to set the chunk options `out.width='100%'` and `out.height='1000px'`:

```
knitr::include_graphics("figures/sample-content/pdf_embed_example/Lyngs2020_FB.pdf")
```

In LaTeX output, however, this approach can cause odd behaviour. Therefore, when you build your thesis to PDF, split the PDF into an alphanumerically sorted sequence of **single-page** PDF files (you can do this automatically with the package `pdftools`). You can then use the appropriate LaTeX command to insert them, as shown below (for brevity, in the `oxforddown` PDF sample content we’re only including two pages). *Note that the chunk option `results='asis'` must be set.* You may also want to remove margins from the PDF files, which you can do with Adobe Acrobat (paid version) and likely other software.

```
# install.packages(pdftools)
# split PDF into pages stored in
  figures/sample-content/pdf_embed_example/split/
#
  pdftools::pdf_split("figures/sample-content/pdf_embed_example/Lyngs2020_FB.pdf")
# output = "figures/sample-content/pdf_embed_example/split/"
# grab the pages
```

5. Customisations and extensions

```
pages <- list.files("figures/sample-content/pdf_embed_example/split",
  full.names = TRUE)

# set how wide you want the inserted PDFs to be:
# 1.0 is 100 per cent of the oxforddown PDF page width;
# you may want to make it a bit bigger
pdf_width <- 1.2

# for each PDF page, insert it nicely and
# end with a page break
cat(stringr::str_c("\\newpage \\begin{center}
  \\makebox[\\linewidth][c]{\\includegraphics[width=", pdf_width,
  "\\linewidth]{", pages, "}} \\end{center}"))
```

‘I Just Want to Hack Myself to Not Get Distracted’: Evaluating Design Interventions for Self-Control on Facebook

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ABSTRACT

Beyond being the world’s largest social network, Facebook is for many also one of its greatest sources of digital distraction. For students, problematic use has been associated with negative effects on academic achievement and general wellbeing. To understand what strategies could help users regain control, we investigated how simple interventions to the Facebook UI affect behaviour and perceived control. We assigned 58 university students to one of three interventions: goal reminders, removed newsfeed, or white background (control). We logged use for 6 weeks, applied interventions in the middle weeks, and administered fortnightly surveys. Both goal reminders and removed newsfeed helped participants stay on task and avoid distraction. However, goal reminders were often annoying, and removing the newsfeed made some fear missing out on information. Our findings point to future interventions such as controls for adjusting types and amount of available information, and flexible blocking which matches individual definitions of ‘distraction’.

Author Keywords

Facebook; problematic use; self-control; distraction; ICT non-use; addiction; focus; interruptions

CCS Concepts

•Human-centered computing → Empirical studies in HCI;

INTRODUCTION

Research on ‘Problematic Facebook Use’ (PFU) has investigated correlations between Facebook use and negative effects on outcomes such as level of academic achievement [35] and subjective wellbeing [58, 57]. A cross-cutting finding is that negative outcomes are associated with difficulty at exerting self-control over use, as well as specific use patterns including viewing friends’ wide-audience broadcasts rather than receiving targeted communication from strong ties [13, 58].

Much of this work has focused on self-control over Facebook use in student populations [2, 44, 46], with media multitasking research finding that students often give in to use which provides short-term ‘guilty pleasures’ over important, but aversive academic tasks [76, 88, 60]. In the present paper, we present a mixed-methods study exploring how two interventions to Facebook — goal reminders and removing the newsfeed — affect university students’ patterns of use and perceived control over Facebook use. To triangulate self-report with objective measurement, our study combined usage logging with fortnightly surveys and post-study interviews.

We found that both interventions helped participants stay on task and use Facebook more in line with their intentions. In terms of use patterns, goal reminders led to less scrolling, fewer and shorter visits, and less time on site, whereas removing the newsfeed led to less scrolling, shorter visits, and less content ‘liked’. However, goal reminders were often experienced as annoying, and removing the newsfeed made some participants fear missing out on information. After the study, participants suggested a range of design solutions to mitigate self-control struggles on Facebook, including controls for filtering or removing the newsfeed, reminders of time spent and of use goals, and removing features that drive engagement. As an exploratory study, this work should be followed by confirmatory studies to assess whether our findings replicate, and how they may generalise beyond a student population.

RELATED WORK

Struggles with Facebook use

Whereas many uses of Facebook offer important benefits, such as social support, rapid spread of information, or facilitation of real-world interactions [78], a substantial amount of research has focused on negative aspects [58]. For example, studies have reported correlations between patterns of Facebook use and lower academic achievement [77, 86], low self-esteem, depression and anxiety [51], feelings of isolation and loneliness [2], and general psychological distress [15]. Such ‘Problematic Facebook Use’ (PFU) has been studied under various names (including ‘Facebook dependence’ [87] and ‘Facebook addiction’ [5]), but a recent review summarised a common definition as ‘problematic behaviour characterised by addictive-like symptoms and/or self-regulation difficulties related to Facebook use leading to negative consequences in personal and social life’ [58].

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CHI ’20, April 25–30, 2020, Honolulu, HI, USA.
© 2020 Copyright is held by the author/owner(s).
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<http://dx.doi.org/10.1145/3313831.3376672>

5. Customisations and extensions

CHI 2020 Paper

CHI 2020, April 25–30, 2020, Honolulu, HI, USA

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5.8 Including another paper in your thesis - R Markdown child document

Sometimes you want to include another paper you are currently writing as a chapter in your thesis. Above 5.7, we described the simplest way to do this: include the other paper as a pdf. However, in some cases you instead want to include the R Markdown source from this paper, and have it compiled within your thesis. This is a little bit more tricky, because you need to keep careful track of your file paths, but it is possible by [including the paper as a child document](#). There are four main steps:

1. Include the paper as a child document
2. Make file paths compatible with knitting the article on its own, as well as when it's include in your thesis
3. Make header levels correct
4. Make figure widths correct

5.8.1 An example paper in another folder

Take this simple example (files for this are in [this GitHub repository](#)):

```
|--paper_to_include
|   |--my_paper.Rmd
|   |--data
|   |   |--cat_salt.csv
|   |--figures
|   |   |--cat.jpg
|
|--thesis
```

As the chart suggests, you have another folder, **paper_to_include/** living in the same containing folder as your thesis folder. In the **paper_to_include** folder, the file **my_paper.Rmd** is where you write the paper. In **my_paper.Rmd**,

5. Customisations and extensions

you read in a CSV file found in the subfolder **data/cats.csv**, and also an image from the subfolder **figures/cat.jpg**.

5.8.2 Step 1: Include paper as a child document

In your thesis folder, create an Rmd file for the chapter where you want to include another paper. Add one or more code chunks that include R Markdown files from that paper as child documents:

```
# Including an external chapter

```{r child = "../paper_to_include/my_paper.Rmd"}
```
```

5.8.3 Step 2: Make file paths compatible

Use [parameters](#) to adjust the file path of images based on values you set in the YAML header of an R Markdown file. In **my_paper.Rmd**, create a parameter called **other_path** and set it to an empty string:

```
---
title: "A fabulous article in a different folder"
params:
  other_path: ""
---
```

In **my_paper.Rmd**, put this at the start of the filepath when you read in data or include images:

```
library(tidyverse)
library(knitr)

cat_data <- read_csv(str_c(params$other_path, "data/cats.csv"))
include_graphics(str_c(params$other_path, "figures/cat.jpg"))
```

5. Customisations and extensions

Finally, in your thesis folder's **index.Rmd** file, also create the parameter **other_path**. But here, set it to where the **paper_to_include/** folder is relative to your thesis folder:

```
params:
  other_path: "../paper_to_include/"
```

Note on HTML output

Note that if you want to host an HTML version on your thesis online, you will need to include graphics in the content that you host online - the internet obviously won't be able to see filepaths that are just referring to stuff in another folder on your computer!

5.8.4 Step 3: Make sure header levels are correct

Unless the paper you want to include is also written as a book, your header levels are probably going to be off. That is, the level 1 headers (# Some header) you use for main sections in the other paper turns into chapter titles when included in your thesis.

To avoid this, first *increment all heading levels by one in **paper_to_include/my_paper.Rmd*** (# Some header -> ## Some header). Then in **paper_to_include/** create a [lua filter](#) that decrements header levels by one: Create a text file, save it as **reduce_header_level.lua**, and give it the content below.

```
function Header(el)
  if (el.level <= 1) then
    error("I don't know how to decrease the level of h1")
  end
  el.level = el.level - 1
  return el
end
```

In the YAML header of **paper_to_include/my_paper.Rmd**, use this filter:

5. Customisations and extensions

```
---  
title: "A fabulous article in a different folder"  
params:  
  other_path: ""  
output:  
  pdf_document:  
    pandoc_args: ["--lua-filter=reduce_header_level.lua"]  
---
```

Now, your header levels will be correct both when you knit the paper on its own and when its included in your thesis.

NOTE: There might be no need to use a lua filter to shift heading - it seems you could simply use `pandoc_args: ["--shift-heading-level-by=-1"]` (see <https://pandoc.org/MANUAL.html#reader-options>)

5.8.5 Step 4. Make sure figure widths are correct

It might be that your figure widths when knitting your paper on its own, and when including it in your thesis, need to be different. You can again use parameters to set figure widths.

Imagine you want figure width to be 80% of the page width when knitting your paper on its own, but 100% in your thesis. In `paper__to__include/my_paper.Rmd`, first add a parameter we could call `out_width` and set it to the string "80%":

```
---  
title: "A fabulous article in a different folder"  
params:  
  other_path: ""  
  out_width: "80%"  
output:  
  pdf_document:
```

5. Customisations and extensions

```
pandoc_args: ["--lua-filter=reduce_header_level.lua"]  
---
```

Then, make sure use that parameter to set the output width when you include figures in `paper_to_include/my_paper.Rmd`:

```
```{r, out.width=params$out_width, fig.cap="A very funny cat"}  
include_graphics(str_c(params$other_path, "figures/cat.jpg"))
```
```

Finally, create the parameter `out_width` in your thesis' `index.Rmd` file:

```
params:  
  other_path: "../paper_to_include/"  
  out_width: "80%"
```

Now, the output width of your figure will be 80% when knitting your paper on its own, and 100% when knitting it as child document of your thesis.

5.9 Customizing referencing

5.9.1 Using a .csl file with pandoc instead of biblatex

The `oxforddown` package uses `biblatex` in LaTeX for referencing. It is also possible to use `pandoc` for referencing by providing a `.csl` file in the YAML header of `index.Rmd` (likely requiring commenting out the `biblatex` code in `templates/template.tex`). This may be helpful for those who have a `.csl` file describing the referencing format for a particular journal. However, note that this approach does not support chapter bibliographies (see Section 5.9.2).

```
csl: ecology.csl
```

5.9.2 Customizing biblatex and adding chapter bibliographies

This section provides one example of customizing `biblatex`. Much of this code was combined from searches on Stack Exchange and other sources (e.g. [here](#)).

5. Customisations and extensions

In `templates/template.tex`, one can replace the existing biblatex calls with the following to achieve referencing that looks like this:

(Charmantier and Gienapp 2014)

Charmantier, A. and P. Gienapp (2014). Climate change and timing of avian breeding and migration: evolutionary versus plastic changes. *Evolutionary Applications* 7(1):15–28. doi: 10.1111/eva.12126.

```
\usepackage[backend=biber,  
  bibencoding=utf8,  
  refsection=chapter, % referencing by chapter  
  style=authoryear,  
  firstinits=true,  
  isbn=false,  
  doi=true,  
  url=false,  
  eprint=false,  
  related=false,  
  dashed=false,  
  clearlang=true,  
  maxcitenames=2,  
  mincitenames=1,  
  maxbibnames=10,  
  abbreviate=false,  
  minbibnames=3,  
  uniquelist=minyear,  
  sortcites=true,  
  date=year  
{biblatex}  
\AtEveryBibitem{%  
  \clearlist{language}%
```

5. Customisations and extensions

```

\clearfield{note}
}

\DeclareFieldFormat{titlecase}{\MakeTitleCase{#1}}

\newrobustcmd{\MakeTitleCase}[1]{%
  \ifthenelse{\ifcurrentfield{booktitle}\OR\ifcurrentfield{booksubtitle}%
    \OR\ifcurrentfield{maintitle}\OR\ifcurrentfield{mainsubtitle}%
    \OR\ifcurrentfield{journaltitle}\OR\ifcurrentfield{journalsubtitle}%
    \OR\ifcurrentfield{issuetitle}\OR\ifcurrentfield{issuesubtitle}%
    \OR\ifentrytype{book}\OR\ifentrytype{mvbook}\OR\ifentrytype{bookinbook}%
    \OR\ifentrytype{booklet}\OR\ifentrytype{suppbook}%
    \OR\ifentrytype{collection}\OR\ifentrytype{mvcollection}%
    \OR\ifentrytype{suppcollection}\OR\ifentrytype{manual}%
    \OR\ifentrytype{periodical}\OR\ifentrytype{suppperiodical}%
    \OR\ifentrytype{proceedings}\OR\ifentrytype{mvproceedings}%
    \OR\ifentrytype{reference}\OR\ifentrytype{mvreference}%
    \OR\ifentrytype{report}\OR\ifentrytype{thesis}}
  {#1}
  {\MakeSentenceCase{#1}}}

% \renewbibmacro{in:}{}
% suppress "in" for articles
%
\renewbibmacro{in:}{%
  \ifentrytype{article}{}{\printtext{\bibstring{in}\intitlepunct}}
  %-- no "quotes" around titles of chapters/article titles
\DeclareFieldFormat[article, inbook, incollection, inproceedings, misc, thesis, unp
{title}{#1}
%-- no punctuation after volume

```

5. Customisations and extensions

```
\DeclareFieldFormat[article]
{volume}{{#1}}
%-- puts number/issue between brackets
\DeclareFieldFormat[article, inbook, incollection, inproceedings, misc, thesis, unp
{number}{\mkbibparens{#1}}
%-- and then for articles directly the pages w/o any "pages" or "pp."
\DeclareFieldFormat[article]
{pages}{#1}
%-- for some types replace "pages" by "p."
\DeclareFieldFormat[inproceedings, incollection, inbook]
{pages}{p. #1}
%-- format 16(4):224--225 for articles
\renewbibmacro*{volume+number+eid}{
  \printfield{volume}%
  \printfield{number}%
  \printunit{\addcolon}
}
```

If you would like chapter bibliographies, in addition insert the following code at the end of each chapter, and comment out the entire REFERENCES section at the end of template.tex.

```
\printbibliography[segment=\therefsection,heading=subbibliography]
```

5.10 Customizing the page headers and footers (PDF)

This can now be done directly in **index.Rmd**'s YAML header. If you are a LaTeX expert and need further customisation that what's currently provided, you can tweak the relevant sections of **templates/template.tex** - the relevant code is beneath the line that begins `\usepackage{fancyhdr}`.

5.11 Diving in to the OxThesis LaTeX template (PDF)

For LaTeX minded people, you can read through `templates/template.tex` to see which additional customisation options are available as well as `templates/ociamthesis.cls` which supplies the base class. For example, `template.tex` provides an option for master’s degree submissions, which changes identifying information to candidate number and includes a word count. At the time of writing, you must set this directly in `template.tex` rather than from the YAML header in `index.Rmd`.

5.12 Customising to a different university

5.12.1 The minimal route

If the front matter in the OxThesis LaTeX template is suitable to your university, customising `oxforddown` to your needs could be as simple as putting the name of your institution and the path to your university’s logo in `index.Rmd`:

```
university: University of You
university-logo: figures/your-logo-here.pdf
```

5.12.2 Replacing the entire title page with your required content

If you have a `.tex` file with some required front matter from your university that you want to replace the OxThesis template’s title page altogether, you can provide a filepath to this file in `index.Rmd`. `oxforddown`’s sample content includes an example of this — if you use the YAML below, your front matter will look like this:

```
alternative-title-page: front-and-back-matter/alt-title-page-example.tex
```


5. Customisations and extensions

| | | |
|--|---|--|
| <p>Title of your Thesis</p> <p>John Doe</p> | <p>Thesis committee</p> <p>Promotor:
Prof.dr. J. Smith
Professor of Geo-information Science and Remote Sensing
Wageningen University</p> <p>Co-promotors:
Dr. Name of co-promotor
Assistant Professor, Laboratory of Geo-information Science and Remote Sensing
Wageningen University</p> <p>Other members:
Prof.dr. Jury member 1, Wageningen University
Prof.dr. Jury member 2, Affiliation
Prof.dr. Jury member 3, Affiliation
Prof.dr. Jury member 4, Affiliation</p> <p>This research was conducted under the auspices of the C.T. de Wit Graduate School of Production Ecology & Resource Conservation (PERC)</p> | <p>Title of your thesis</p> <p>John Doe</p> <p>Thesis
submitted in fulfillment of the requirements for the degree of doctor at
Wageningen University
by the authority of the Rector Magnificus
Prof. Dr A.P.J. Mol,
in the presence of the
Thesis Committee appointed by the Academic Board
to be defended in public
on Date of your defense
at 4 p.m. in the Aula</p> |
| <p>John Doe
Title of your thesis
77 pages
PhD thesis, Wageningen University, Wageningen, NL (2015)
With references, with summary in English
ISBN XXX-YYY</p> | <p>For Yihai Xie</p> | <p>Acknowledgements</p> <p>This is where you will normally thank your advisor, colleagues, family and friends, as well as funding and institutional support. In our case, we will give our thanks to the people who developed the ideas and tools that allow us to push open science a little step forward by writing plain-text, transparent, and reproducible theses in R Markdown.</p> <p>We must be grateful to John Gruber for inventing the original version of Markdown, to John MacFarlane for creating Pandoc (http://pandoc.org) which converts Markdown to a large number of output formats, and to Yihai Xie for creating <code>knitr</code> which introduced R Markdown as a way of embedding code in Markdown documents, and <code>bookdown</code> which added tools for technical and longer-form writing.</p> <p>Special thanks to Chetani Ismay, who created the <code>thesisdown</code> package that helped many a PhD student write their theses in R Markdown. And a very special thanks to John MacFarlane, whose adoption of Stan Evans' adaptation of Keith Gilmer's original <code>muth</code> template for writing an Oxford University DPhil thesis in L^AT_EX provided the template that I in turn adapted for R Markdown.</p> <p>Finally, profuse thanks to JJ Allaire, the founder and CEO of RStudio, and Hadley Wickham, the mastermind of the <code>tidyverse</code> without whom we'd all just given up and done data science in Python instead. Thanks for making data science easier, more accessible, and more fun for us all.</p> <p>Ulrik Lemp
Linacre College, Oxford
2 December 2018</p> |

6

Troubleshooting

This chapter describes common errors you may run into, and how to fix them.

6.1 Error: Failed to build the bibliography via biber

This can happen if you've had a failed build, perhaps in relation to RStudio shutting down abruptly.

Try doing this:

1. type `make clean-knits` in the terminal tab (or run `file.remove(list.files(pattern = "*.log|mtc|maf|aux|bbl|blg|xml"))` in the R console) to clean up files generated by LaTeX during a build
2. restart your computer

If this does not solve the problem, try using the [natbib](#) LaTeX package instead of [biblatex](#) for handling references. To do this, go to **index.Rmd** and

1. set `use-biblatex: false` and `use-natbib: true`
2. set `citation_package: natbib` under

6. *Troubleshooting*

```
output:
```

```
  bookdown::pdf_book:
```

```
    citation_package: natbib
```

*Alles Gescheite ist schon gedacht worden.
Man muss nur versuchen, es noch einmal zu denken.
All intelligent thoughts have already been thought;
what is necessary is only to try to think them again.*

— Johann Wolfgang von Goethe
[von_goethe_wilhelm_1829]

Conclusion

If we don't want Conclusion to have a chapter number next to it, we can add the `{-}` attribute.

More info

And here's some other random info: the first paragraph after a chapter title or section head *shouldn't be* indented, because indents are to tell the reader that you're starting a new paragraph. Since that's obvious after a chapter or section title, proper typesetting doesn't add an indent there.

This paragraph, by contrast, *will* be indented as it should because it is not the first one after the 'More info' heading. All hail LaTeX. (If you're reading the HTML version, you won't see any indentation - have a look at the PDF version to understand what in the earth this section is babbling on about).

7

Methods

Contents

| | |
|------------------------|----|
| 7.1 Datasets | 68 |
|------------------------|----|

7.1 Datasets

The primary dataset of heme-containing proteins (HEM) was composed by searching for proteins containing “HEM” in the PDB. 58 PDBs were kept after culling a much larger list. Not all PDBs were suitable for the investigation - some contain two ligands in one pocket, or two proteins per PDB (IDK HOw to say this properly rn)

A similar culling was done for the other ligands. From this work we ended up with the following dataset sizes: HEM 58, HEC ...

Notes for each dataset.

8

Results

Trial

Here we'll attempt to use the `r` block of code to show a dataframe to the right. And there we are. In the future I should find if there's a more reproducible solution than just saving the global environment to a data file. Perhaps if I could just be like `main.R` and then call stuff. But that takes FOREVER to run, so this for now.

| Residue | Freq |
|---------|------|
| LEU | 8 |
| ALA | 7 |
| TYR | 7 |
| GLY | 6 |
| SER | 6 |
| ARG | 5 |
| HIS | 5 |
| PHE | 5 |
| VAL | 5 |
| GLU | 4 |
| LYS | 4 |
| ASN | 3 |
| GLN | 3 |
| ILE | 3 |
| MET | 3 |
| THR | 3 |
| ASP | 2 |

Appendices



Figures

A.1 AA Frequency

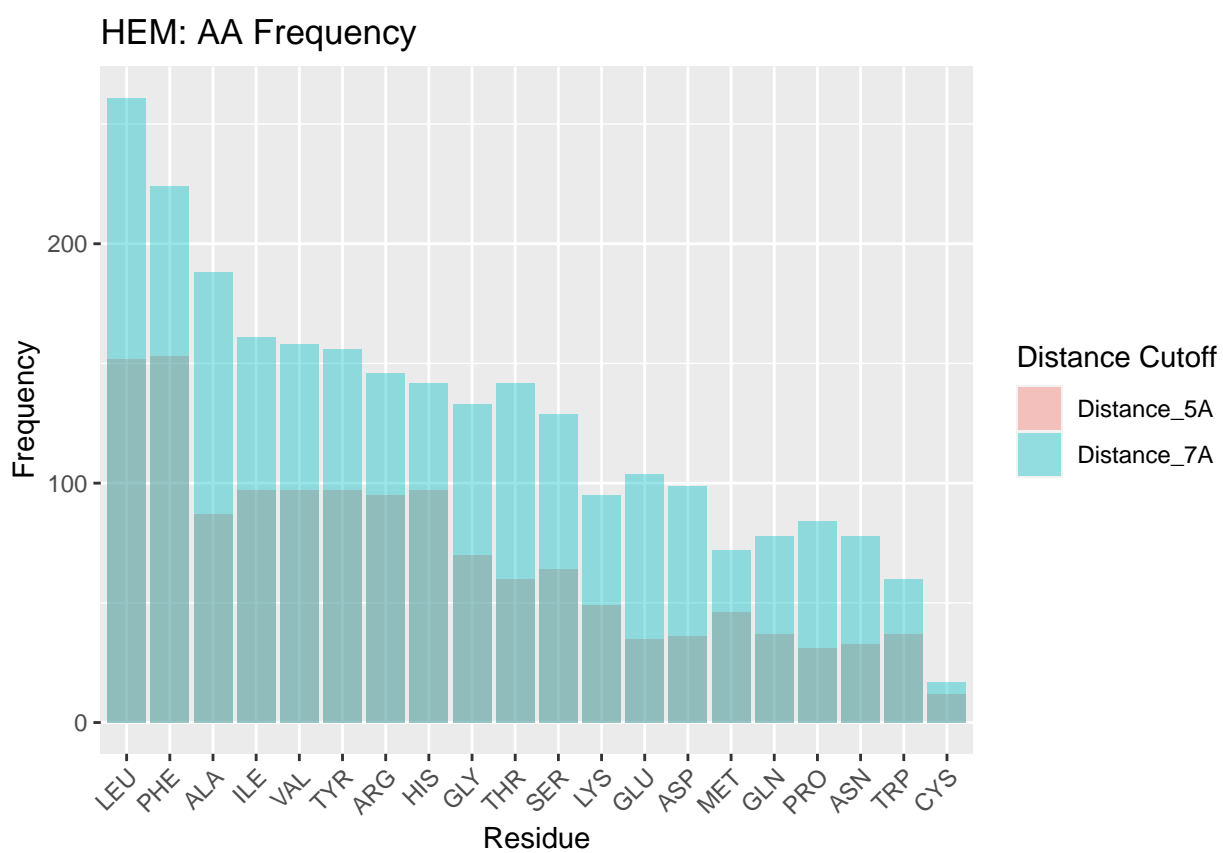


Figure A.1: HEM: AA Frequency

A. Figures

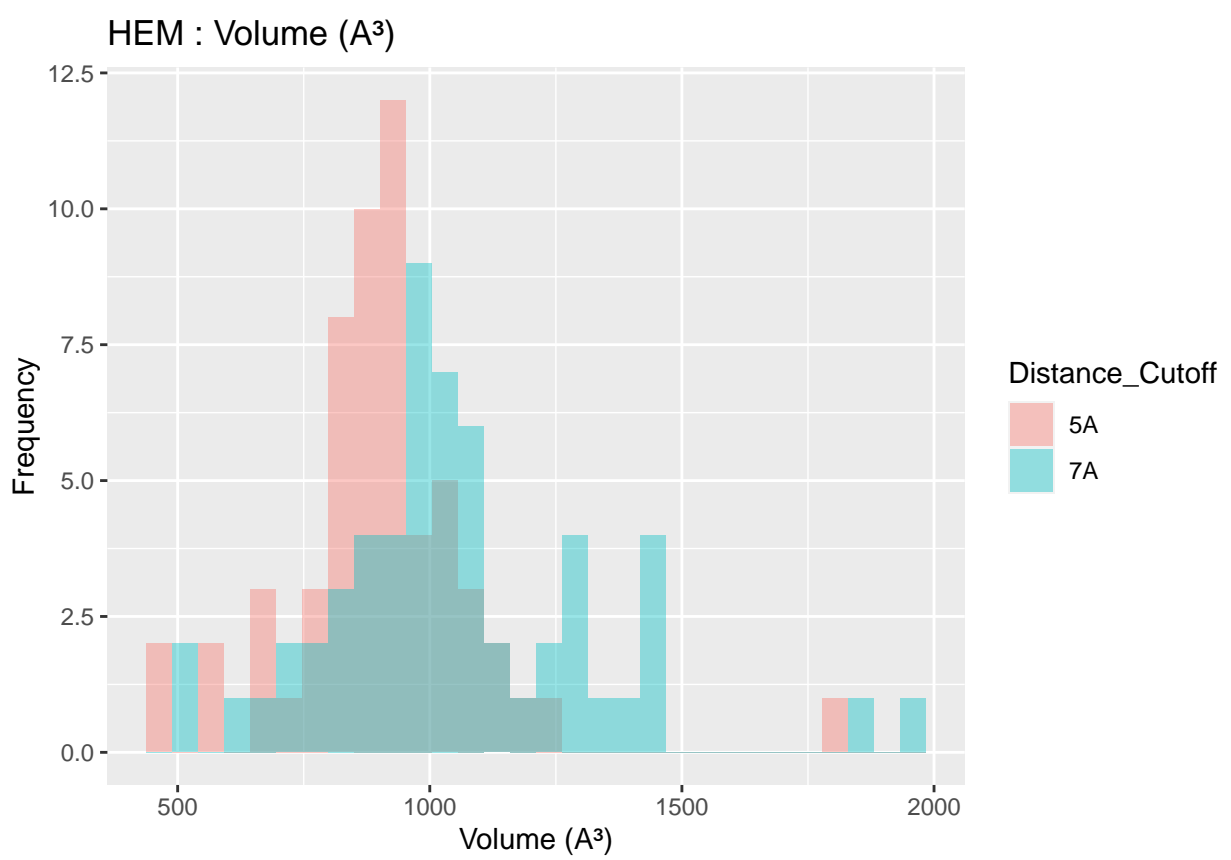


Figure A.2: HEM: Volume

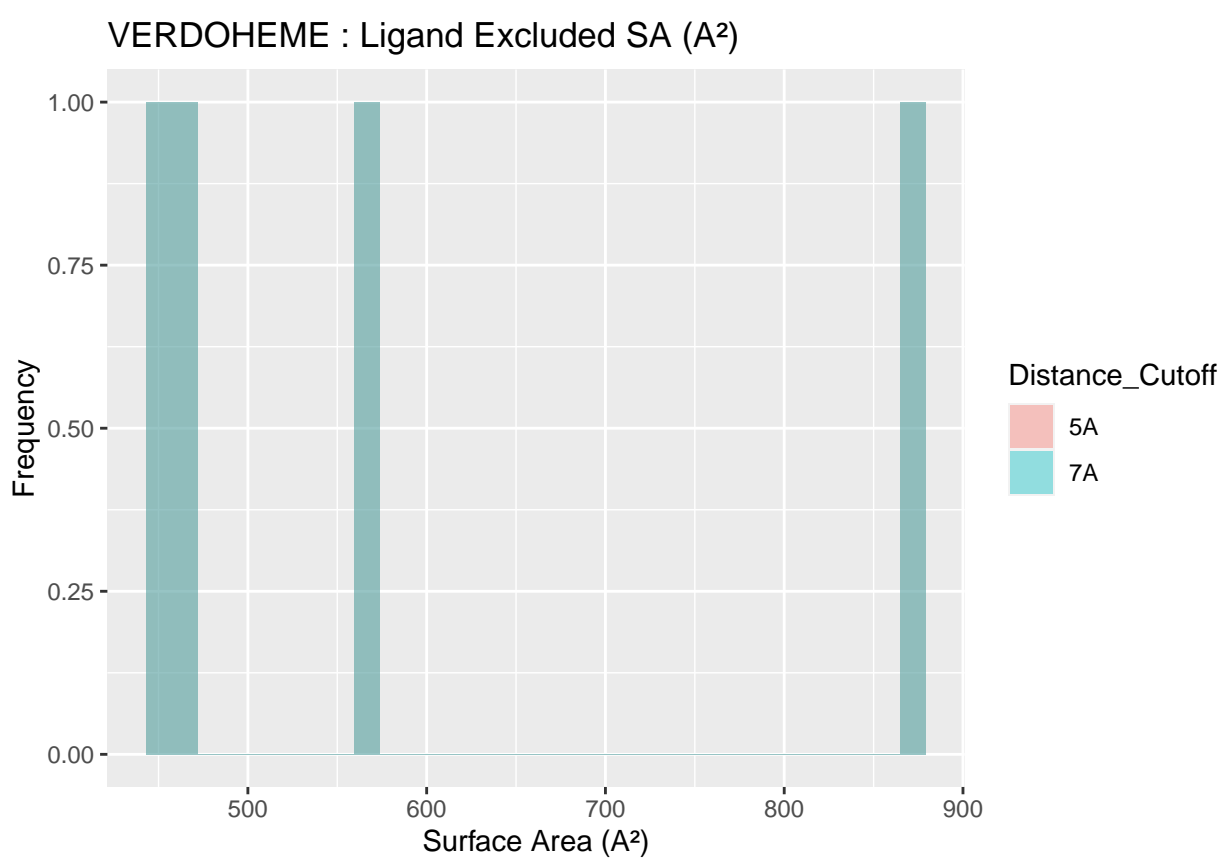


Figure A.3: HEM: Ligand Excluded Surface Area

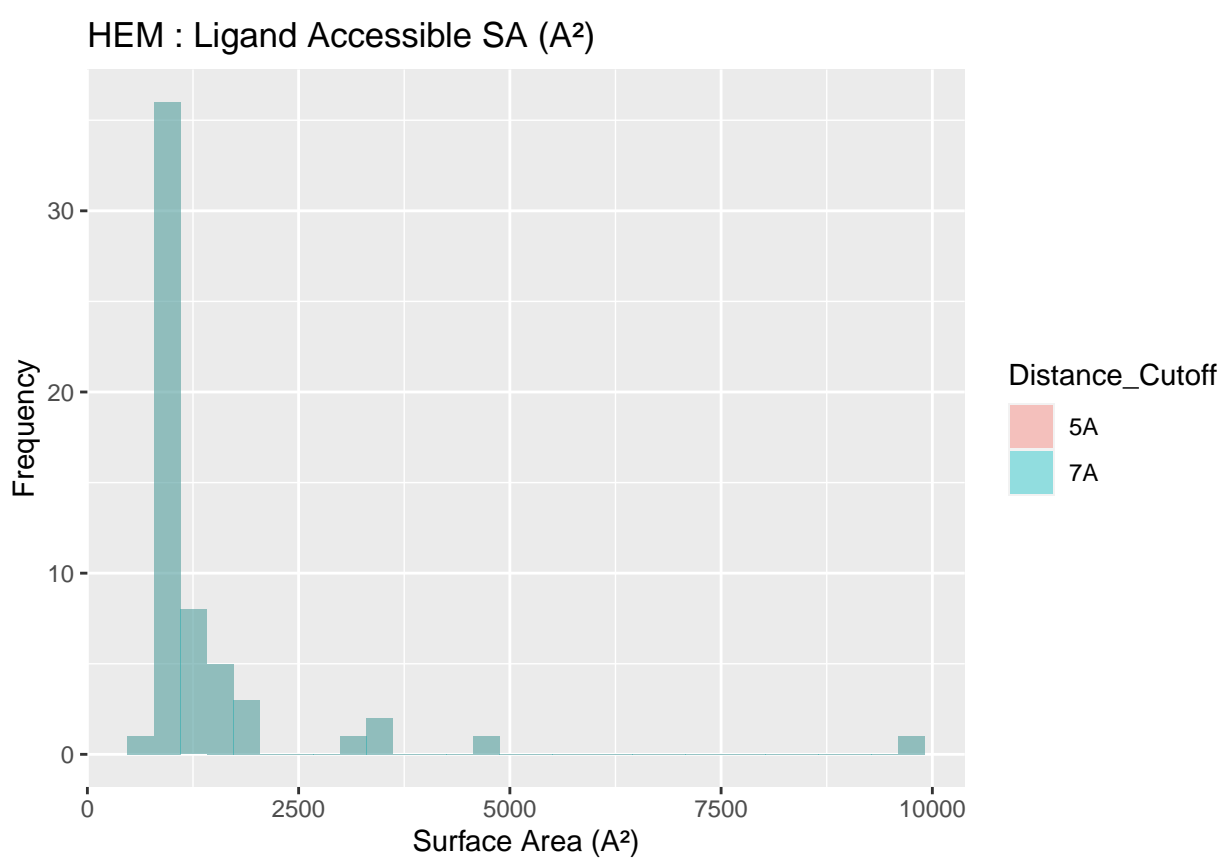


Figure A.4: HEM: Ligand Accessible Surface Area

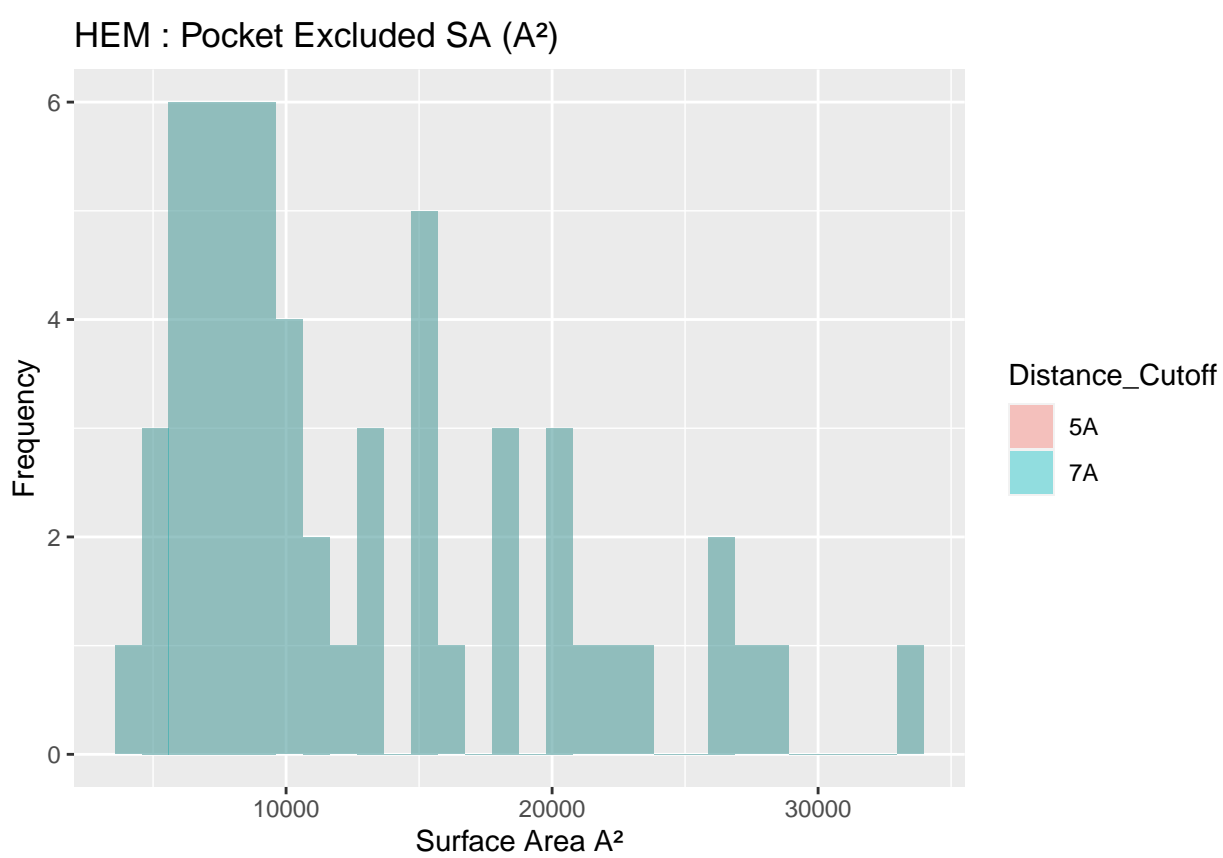


Figure A.5: HEM: Pocket Excluded Surface Area

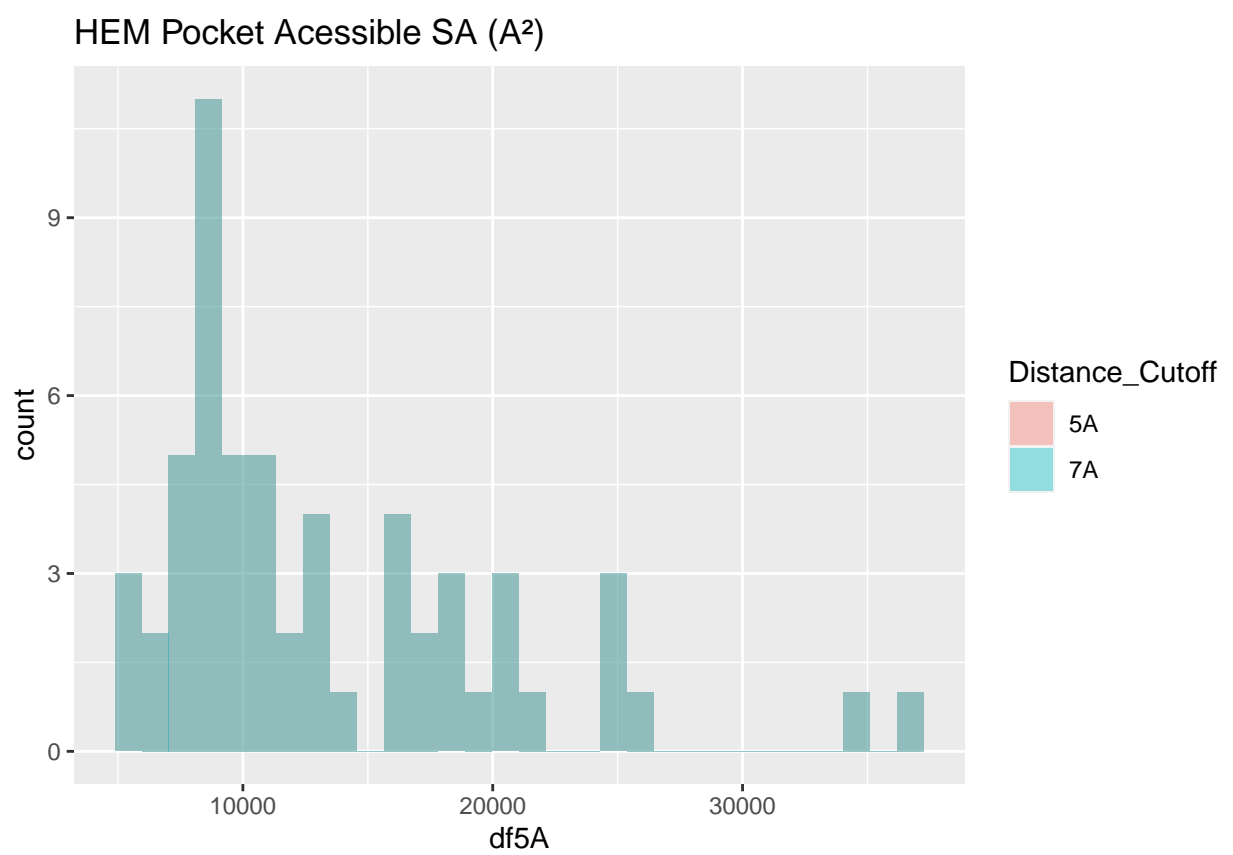


Figure A.6: HEM: Pocket Accessible Surface Area

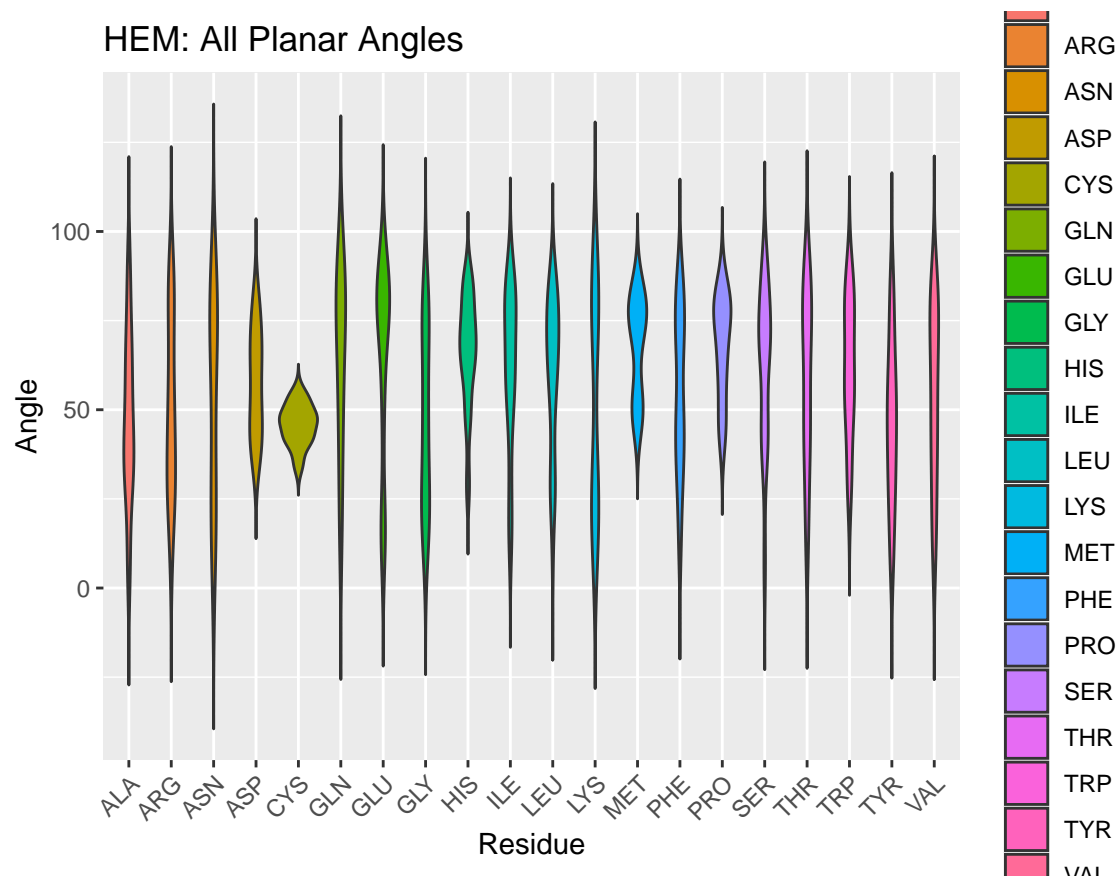


Figure A.7: HEM: All Planar Angles



Figure A.8: HEM: Planar Angles of Closest Residues

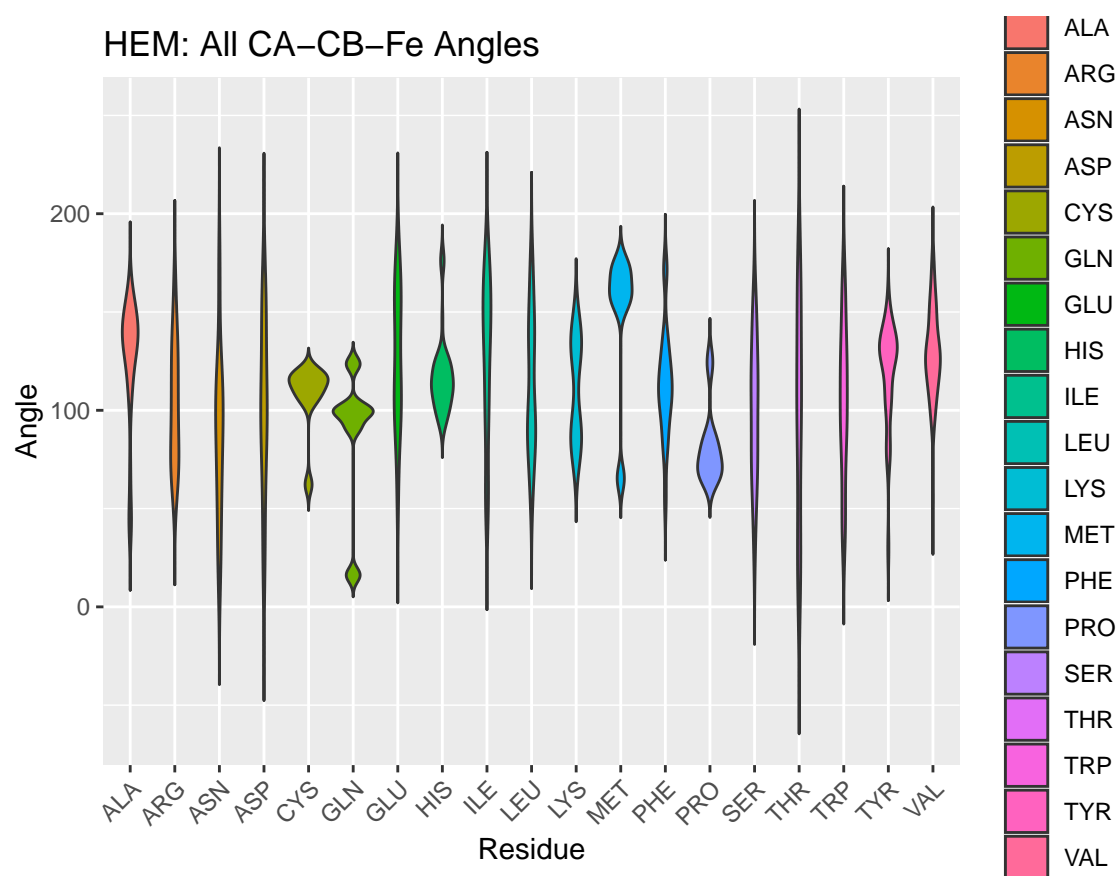


Figure A.9: HEM: All CACBFe Angles

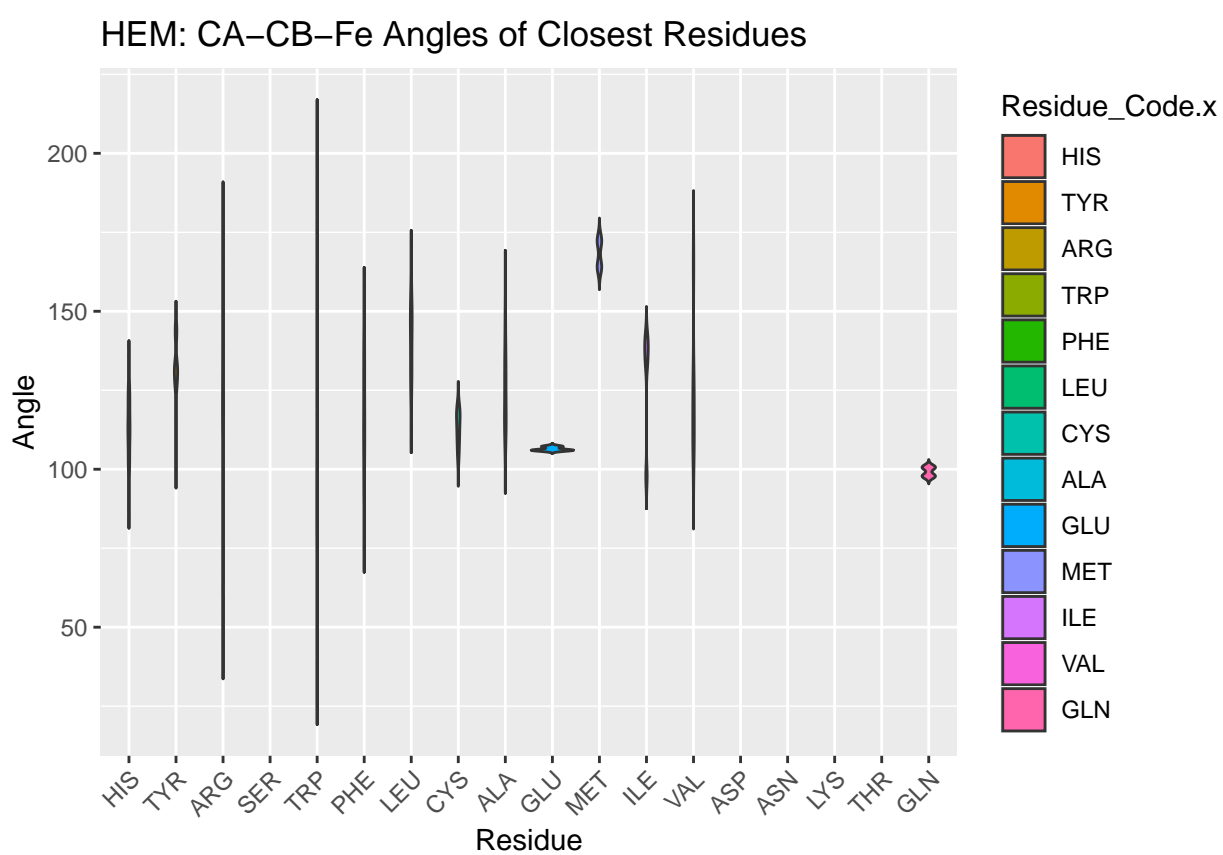


Figure A.10: HEM: Closest CACBFe Angles

B

Tables

B.1 Molecule Names and Source Organisms

Table B.1: HEMp1DF

| PDB_ID | Molecule_Name | Source_Organism |
|--------|---|----------------------------|
| 1B2V | PROTEIN
(HEME-BINDING
PROTEIN A); | SERRATIA
MARCESCENS; |
| 1B5M | CYTOCHROME B5; | RATTUS
NORVEGICUS; |
| 1DK0 | HEME-BINDING
PROTEIN A; | SERRATIA
MARCESCENS; |
| 1DKH | HEME-BINDING
PROTEIN A; | SERRATIA
MARCESCENS; |
| 1ICC | CYTOCHROME B5
OUTER
MITOCHONDRIAL
MEMBRANE | RATTUS
NORVEGICUS; |
| 1IPH | CATALASE HP1I; | ESCHERICHIA COLI; |
| 1N45 | HEME OXYGENASE 1; | HOMO SAPIENS; |
| 1P3T | HEME OXYGENASE 1; | NEISSERIA
MENINGITIDIS; |

Table B.1: HEMp1DF (*continued*)

| PDB_ID | Molecule_Name | Source_Organism |
|--------|--|--|
| 1QHU | PROTEIN | ORYCTOLAGUS |
| 1QJS | (HEMOPEXIN);
HEMOPEXIN; | CUNICULUS;
ORYCTOLAGUS
CUNICULUS; |
| 1SI8 | CATALASE; | ENTEROCOCCUS |
| 1SY2 | NITROPHORIN 4; | FAECALIS;
RHODNIUS |
| 1U9U | CYTOCHROME B5; | PROLIXUS;
BOS TAURUS; |
| 1VGI | HEME OXYGENASE 1; | RATTUS
NORVEGICUS; |
| 1ZVI | NITRIC-OXIDE
SYNTHASE, BRAIN; | RATTUS
NORVEGICUS; |
| 2BHJ | NITRIC OXIDE
SYNTHASE; | MUS MUSCULUS; |
| 2CJ0 | CHLOROPEROXIDASE; | CALDARIOMYCES
FUMAGO; |
| 2CN4 | HEMOPHORE HASA; | SERRATIA
MARCESCENS; |
| 2CPO | CHLOROPEROXIDASE; | LEPTOXYPHIUM
FUMAGO; |
| 2E2Y | MYOGLOBIN; | PHYSETER
CATODON; |
| 2FC2 | NITRIC OXIDE
SYNTHASE; | BACILLUS SUBTILIS; |
| 2IIZ | MELANIN
BIOSYNTHESIS
PROTEIN TYRA,
PUTATIVE; | SHEWANELLA
ONEIDENSIS; |
| 2IPS | LACTOPEROXIDASE; | BOS TAURUS; |
| 2J0P | HEMIN TRANSPORT
PROTEIN HEMS; | YERSINIA
ENTEROCOLITICA; |
| 2J18 | CHLOROPEROXIDASE; | CALDARIOMYCES
FUMAGO; |
| 2O6P | IRON-REGULATED
SURFACE
DETERMINANT
PROTEIN C; | STAPHYLOCOCCUS
AUREUS SUBSP.
AUREUS; |

Table B.1: HEMp1DF (*continued*)

| PDB_ID | Molecule_Name | Source_Organism |
|--------|--|-----------------------------------|
| 2Q6N | CYTOCHROME P450 | ORYCTOLAGUS |
| 2R7A | 2B4;
BACTERIAL HEME | CUNICULUS;
SHIGELLA |
| 2SPL | BINDING PROTEIN;
MYOGLOBIN; | DYSENTERIAE;
PHYSETER |
| 2VEB | PROTOGLOBIN; | CATODON;
METHANOSARCINA |
| 3HX9 | PROTEIN RV3592; | ACETIVORANS;
MYCOBACTERIUM |
| 3MVF | NITROPHORIN-4; | TUBERCULOSIS;
RHODNIUS |
| 3QZN | IRON-REGULATED
SURFACE
DETERMINANT | PROLIXUS;
STAPHYLOCOCCUS |
| 3QZZ | PROTEIN A;
METHANOSARCINA
ACETIVORANS | AUREUS SUBSP.
AUREUS; |
| 3SIK | PROTOGLOBIN;
CONSERVED DOMAIN
PROTEIN; | METHANOSARCINA
ACETIVORANS; |
| 3TGC | NITROPHORIN-4; | BACILLUS
ANTHRACIS; |
| 3VP5 | TRANSCRIPTIONAL
REGULATOR; | RHODNIUS
PROLIXUS; |
| 3ZJS | PROTOGLOBIN; | LACTOCOCCUS
LACTIS; |
| 4B8N | CYTOCHROME | METHANOSARCINA
ACETIVORANS; |
| 4CAT | B5-HOST ORIGIN;
CATALASE; | OSTREOCOCCUS
TAURI VIRUS 2; |
| 4CDP | PUTATIVE
HEME/HEMOGLOBIN
TRANSPORT
PROTEIN; | PENICILLIUM
JANTHINELLUM; |
| 4I3Q | CYTOCHROME P450 | ESCHERICHIA COLI; |
| 4JET | 3A4;
HEMOPHORE HASA; | HOMO SAPIENS;
YERSINIA PESTIS; |

Table B.1: HEMp1DF (*continued*)

| PDB_ID | Molecule_Name | Source_Organism |
|--------|---------------------------|--------------------|
| 4MF9 | HEMIN DEGRADING | PSEUDOMONAS |
| 4MYP | FACTOR;
IRON-REGULATED | AERUGINOSA; |
| | SURFACE | LISTERIA |
| | DETERMINANT | MONOCYTOGENES; |
| | PROTEIN A; | |
| 4NL5 | HEME-DEGRADING | MYCOBACTERIUM |
| | MONOOXYGENASE | TUBERCULOSIS; |
| | HMOB; | |
| 4UZV | HEMOGLOBIN; | THERMOBIFIDA |
| | | FUSCA TM51; |
| 4XZD | EXTRACELLULAR | YERSINIA PSEUDOTU- |
| | HEME ACQUISITION | BERCULOSIS IP |
| | HEMOPHORE HASA; | 32953; |
| 4Y1Q | EXTRACELLULAR | YERSINIA PSEUDOTU- |
| | HEME ACQUISITION | BERCULOSIS IP |
| | HEMOPHORE HASA; | 32953; |
| 5CN5 | MYOGLOBIN; | EQUUS CABALLUS; |
| 5GJ3 | PERIPLASMIC | ROSEIFLEXUS SP. |
| | BINDING PROTEIN; | RS-1; |
| 5KZL | HEME OXYGENASE; | LEPTOSPIRA |
| | | INTERROGANS; |
| 5O1L | RUBBER | STREPTOMYCES SP. |
| | OXYGENASE; | (STRAIN K30); |
| 5O1M | RUBBER | STREPTOMYCES SP. |
| | OXYGENASE; | (STRAIN K30); |
| 5VEU | CYTOCHROME P450 | HOMO SAPIENS; |
| | 3A5; | |
| 6A2J | HEME A SYNTHASE; | BACILLUS SUBTILIS |
| | | (STRAIN 168); |
| 7C74 | LACTOPEROXIDASE; | BOS MUTUS; |
| 7DMR | LACTOPEROXIDASE; | BOS MUTUS; |

Table B.2: HEMp2DF

| PDB_ID | Volume_Data | HEM_Excluded_SA | HEM_Accessible_SA | Pocket_Excluded_SA | Pocket_Accessible_SA |
|--------|-------------|-----------------|-------------------|--------------------|----------------------|
| 1B2V | 893.60 | 502.042 | 820.988 | 7276.09 | 8232.60 |
| 1B5M | 672.79 | 490.050 | 800.780 | 4695.01 | 5512.20 |
| 1DK0 | 966.72 | 505.258 | 837.157 | 7237.94 | 8217.58 |
| 1DKH | 1010.70 | 509.042 | 828.131 | 7402.34 | 8175.94 |
| 1ICC | 1000.40 | 499.585 | 811.357 | 5079.72 | 6028.23 |
| 1IPH | 1345.60 | 501.603 | 814.652 | 33983.80 | 34094.40 |
| 1N45 | 978.98 | 560.384 | 983.238 | 9944.50 | 10779.30 |
| 1P3T | 987.05 | 509.939 | 829.611 | 9530.67 | 10410.80 |
| 1QHU | 1389.20 | 573.686 | 1002.160 | 18503.10 | 18257.20 |
| 1QJS | 1102.30 | 573.266 | 1000.380 | 18588.40 | 18584.10 |
| 1SI8 | 965.57 | 646.643 | 1184.070 | 23711.20 | 25120.40 |
| 1SY2 | 918.34 | 501.850 | 817.749 | 8960.76 | 9610.23 |
| 1U9U | 738.55 | 496.132 | 813.773 | 4675.76 | 5632.32 |
| 1VGI | 870.44 | 577.234 | 1002.530 | 9615.29 | 10248.20 |
| 1ZVI | 1435.90 | 701.091 | 1129.540 | 19918.60 | 20968.20 |
| 2BHJ | 1438.30 | 836.576 | 1290.530 | 20102.30 | 20762.60 |
| 2CJ0 | 809.62 | 2653.180 | 4835.280 | 12749.60 | 12892.20 |
| 2CN4 | 526.88 | 576.760 | 961.348 | 9617.23 | 11917.70 |
| 2CPO | 886.17 | 1846.490 | 3329.540 | 13081.60 | 12995.60 |
| 2E2Y | 994.92 | 811.270 | 1607.370 | 7531.94 | 8240.75 |
| 2FC2 | 1091.40 | 1011.190 | 1669.900 | 18383.50 | 18552.10 |
| 2IIZ | 1015.60 | 731.342 | 1393.160 | 13651.70 | 14031.40 |
| 2IPS | 1242.40 | 618.252 | 1075.560 | 27760.50 | 25814.10 |
| 2J0P | 1281.80 | 1030.510 | 1873.810 | 15192.90 | 15871.10 |
| 2J18 | 841.67 | 1962.990 | 3556.340 | 12675.10 | 12779.00 |
| 2O6P | 788.05 | 499.017 | 822.121 | 6234.84 | 7200.43 |
| 2Q6N | 1030.10 | 644.365 | 1040.080 | 20051.10 | 19747.50 |
| 2R7A | 1284.50 | 507.098 | 845.182 | 11255.10 | 12389.00 |
| 2SPL | 1055.70 | 589.706 | 1029.660 | 7588.36 | 8105.94 |
| 2VEB | 886.06 | 762.309 | 1454.750 | 9840.72 | 10401.80 |
| 3HX9 | 1844.50 | 785.442 | 1168.200 | 5819.08 | 7189.03 |
| 3MVF | 1271.40 | 576.502 | 1009.950 | 8559.24 | 9573.08 |
| 3QZN | 726.52 | 664.858 | 1221.330 | 6133.24 | 7179.49 |
| 3QZZ | 977.30 | 496.950 | 825.255 | 8523.59 | 9708.28 |

Table B.2: HEMp2DF (*continued*)

| PDB_ID | Volume_Data | HEM_Excluded_SA | HEM_Accessible_SA | Pocket_Excluded_SA | Pocket_Accessible_SA |
|--------|-------------|-----------------|-------------------|--------------------|----------------------|
| 3SIK | 492.15 | 498.621 | 823.565 | 6495.38 | 7739.06 |
| 3TGC | 969.87 | 524.380 | 853.710 | 8712.77 | 9181.94 |
| 3VP5 | 1094.60 | 602.790 | 1050.820 | 9801.82 | 10810.80 |
| 3ZJS | 788.74 | 528.419 | 860.137 | 9568.10 | 10130.40 |
| 4B8N | 841.27 | 569.302 | 990.216 | 4560.39 | 5458.66 |
| 4CAT | 1933.90 | 484.341 | 778.502 | 28372.40 | 36788.30 |
| 4CDP | 1053.70 | 1425.050 | 3141.090 | 14733.50 | 15887.40 |
| 4I3Q | 1220.50 | 510.623 | 845.108 | 21946.50 | 21093.70 |
| 4JET | 1010.80 | 495.992 | 818.131 | 7887.81 | 8695.85 |
| 4MF9 | 1286.50 | 488.695 | 790.732 | 15669.80 | 16791.30 |
| 4MYP | 610.72 | 963.019 | 1834.680 | 6285.40 | 7351.53 |
| 4NL5 | 1088.70 | 576.669 | 1003.400 | 5715.52 | 6894.72 |
| 4UZV | 1184.10 | 526.584 | 844.058 | 7378.28 | 8322.74 |
| 4XZD | 932.14 | 498.788 | 816.032 | 8028.32 | 8752.50 |
| 4Y1Q | 952.23 | 494.939 | 806.960 | 7905.84 | 8785.04 |
| 5CN5 | 1070.30 | 663.162 | 1223.640 | 7629.45 | 8117.34 |
| 5GJ3 | 1108.20 | 756.603 | 1131.670 | 11394.00 | 12591.80 |
| 5KZL | 914.22 | 483.760 | 805.567 | 9662.03 | 10431.00 |
| 5O1L | 1438.70 | 801.519 | 1447.270 | 15538.20 | 16876.00 |
| 5O1M | 1431.30 | 493.850 | 799.331 | 16096.90 | 15912.50 |
| 5VEU | 964.76 | 993.578 | 1502.660 | 20900.80 | 20425.90 |
| 6A2J | 1015.90 | 6183.450 | 9902.920 | 14870.30 | 15888.00 |
| 7C74 | 1155.10 | 497.527 | 820.381 | 26111.40 | 25094.20 |
| 7DMR | 1083.40 | 1049.750 | 1916.950 | 26004.00 | 24563.80 |

This is an attempt at referencing the tables above.

figure reference ?? table reference [B.2](#)

Works Cited

- [1] Ting Li, Herbert L Bonkovsky, and Jun Tao Guo. “Structural analysis of heme proteins: Implications for design and prediction”. In: *BMC Structural Biology* 11 (2011). DOI: [10.1186/1472-6807-11-13](https://doi.org/10.1186/1472-6807-11-13).