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

TO BE COMPLETED UPON AGREEMENT OF DISCUSSION/CONCLUSION

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.

Contents

List of Figures

List of Tables

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]). The study focused on the structural differences between hemoproteins with bound and unbound ligands.

In this study, structures of hemoproteins with bound ligands were examined. Multiple ligands and their binding protein were examined: heme (HEM), heme-c (HEC), siroheme (SER), and verdoheme (VEA/VER).

Of particular interest were any qualities that may suggest a requirement for ligand binding. In addition, with several ligands studied, the similarities and differences for binding pockets for the different ligands could be elucidated. Properties of the binding pockets were both predicted and observed from their respective PDB files.

0.1 other stuff to consider adding to the introduction

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: XXXXXXXXX.

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

1 How to use

Contents

1.1 How `oxforddown` is structured

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

```
|   +-- _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):

```
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
ordinary-page-number-position: C
...

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

  bookdown::bs4_book:
```

```
    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.

1.1.5 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**

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";
    ...
```

- 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
```

```
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

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

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

Sub_2 and super^2 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. 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 created[1] 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}
```

[1] my footnote text
[2] This is a random test.

Becomes:

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

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.

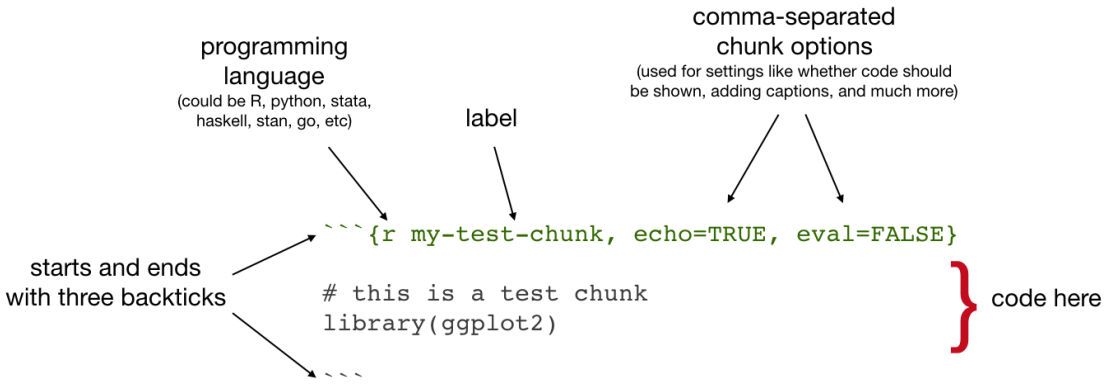

Figure 2.1: Code chunk syntax

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

- `echo`: whether or not to display code in knitted output
- `eval`: whether or to 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 underscoores 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()
```

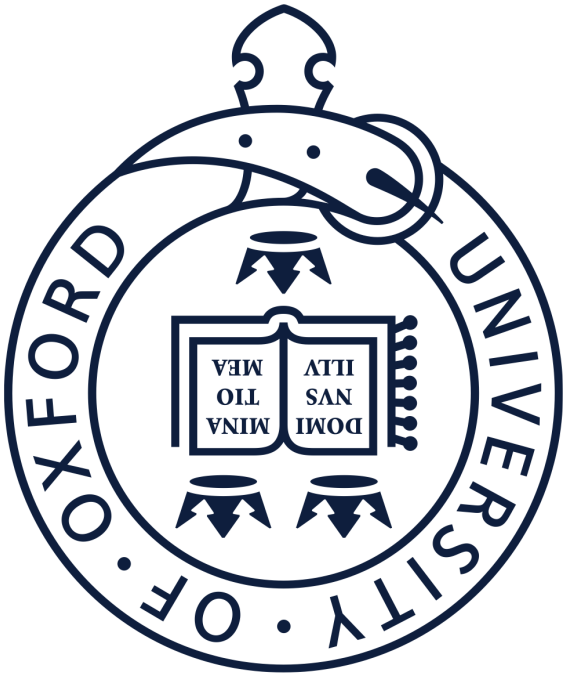

Figure 2.3: Oxford logo, rotated

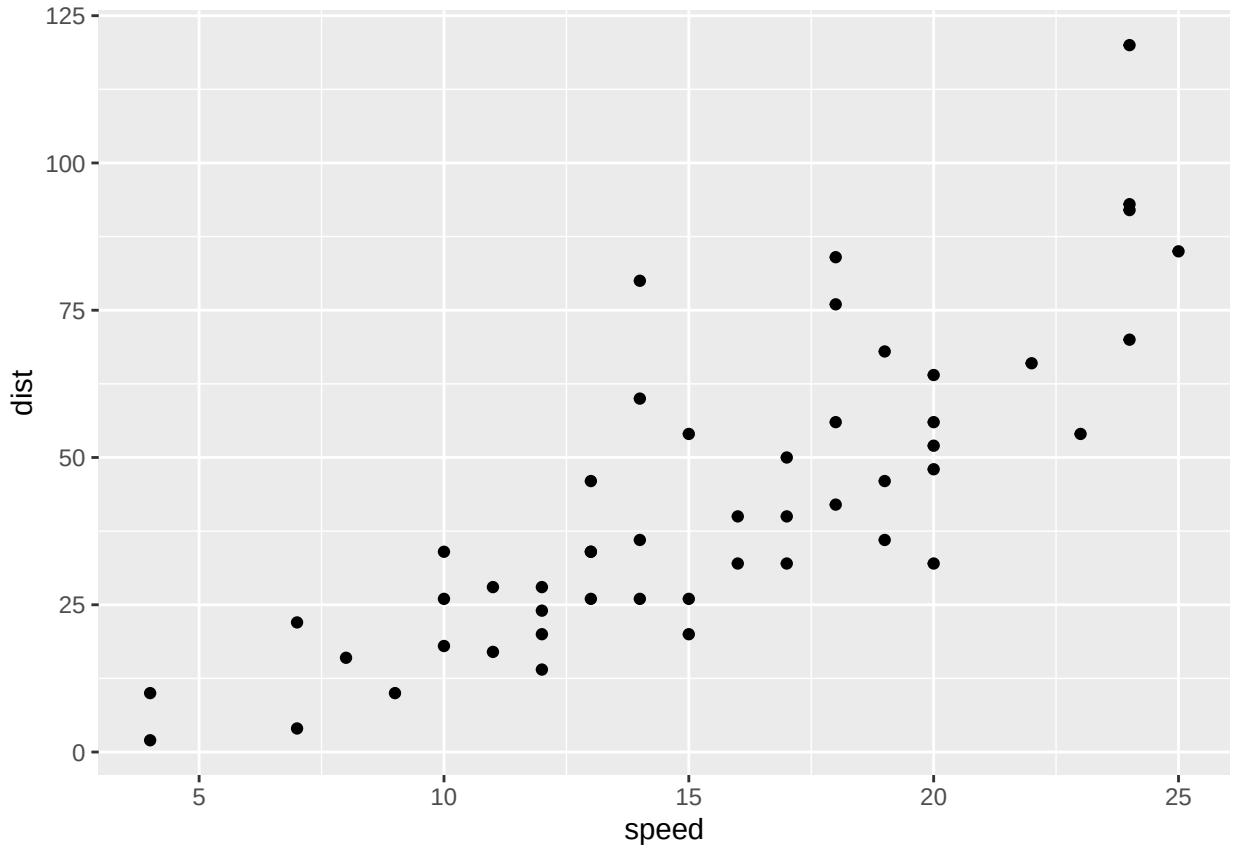

Figure 2.4: A ggplot of car stuff

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:

```
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

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`.

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

Most reference managers can create a .bib file with you 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 highlighed section, 'Shea2014' is the **citation identifier**. To 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)

  - 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.

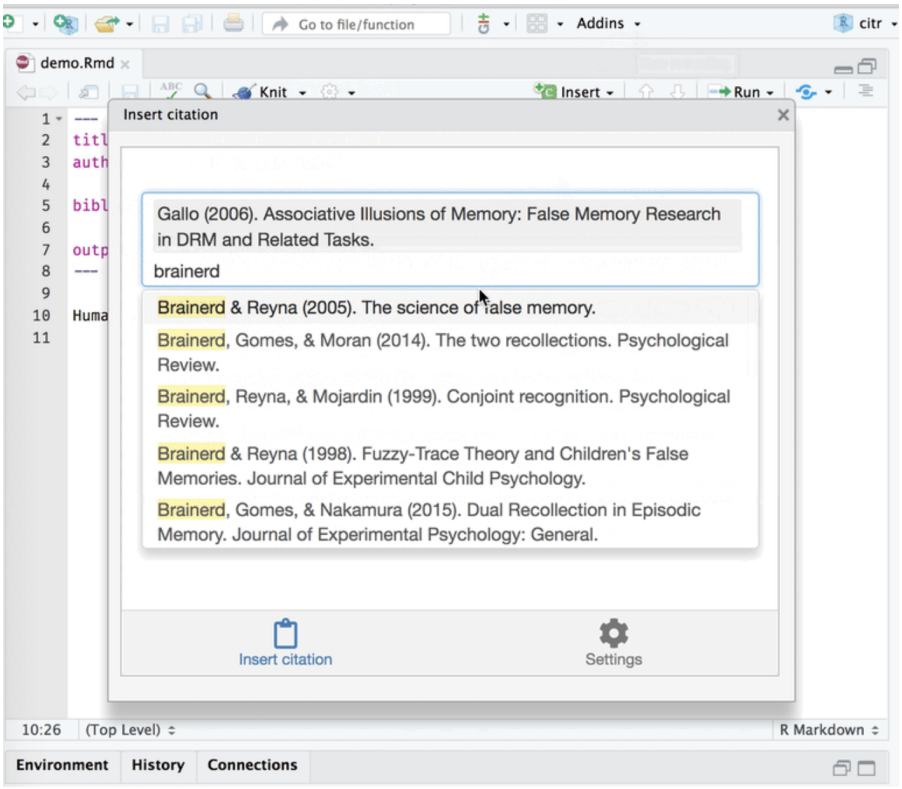

Figure 3.1: The 'citr' add-in

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)`

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:

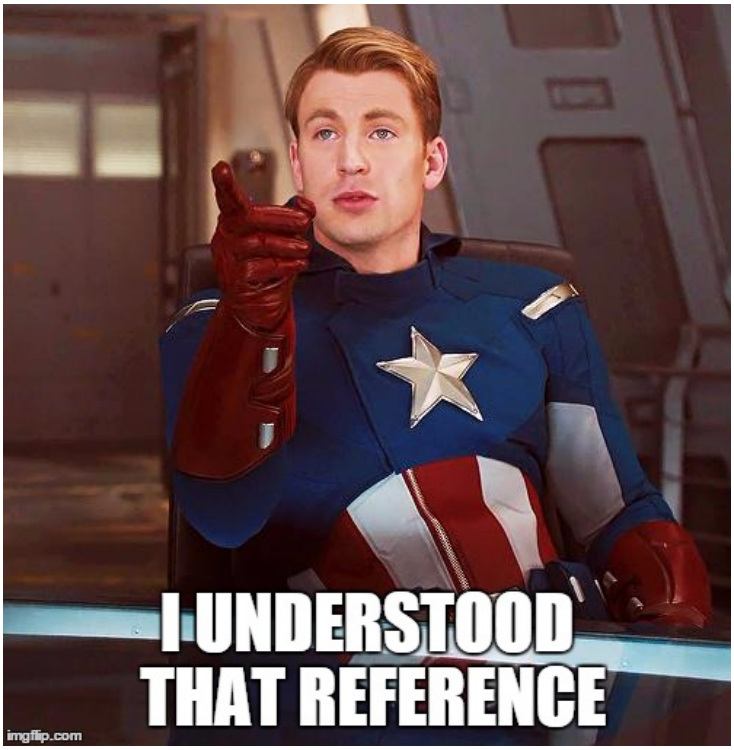

Figure 3.2: A marvel-lous meme

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

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).

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

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:

```
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.

	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

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

Maserati Bora1	15.0	8	301.0	335	3.54	3.570	14.60	0
Volvo 142E1	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

(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:

```
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

(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.

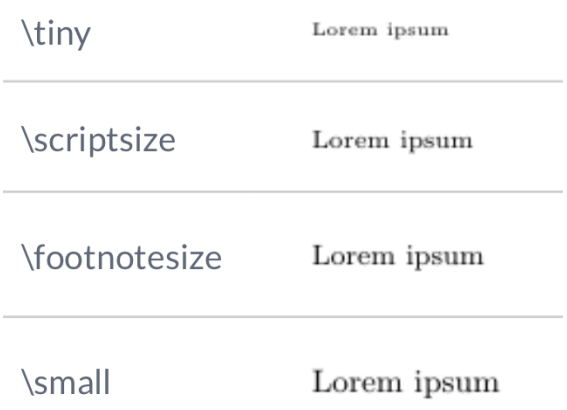

Figure 4.1: Font sizes in LaTeX

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\\}')
```

```
#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
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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
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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

(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

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]

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

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!

5.5.2 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

[2] In 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>`.

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
```

```
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].

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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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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**,

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"))
```

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 chaper 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:

```
---
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:
```

```
    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).

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}%
```

```
  \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
```

```
\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

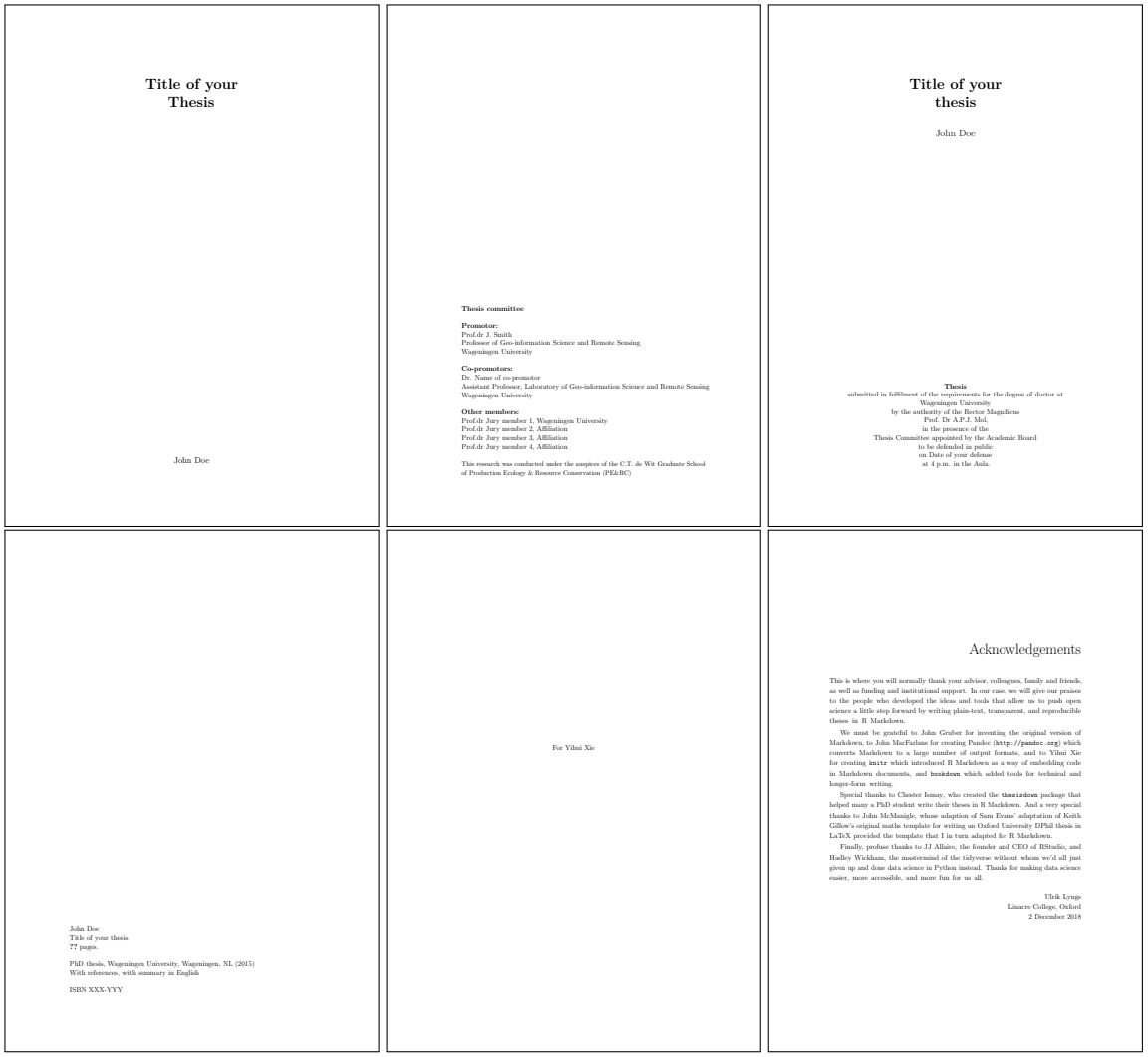
If the front matter in the OxThesis LaTeX template is suitable to your university, customising `oxforddown` to your needs could be as simple as putting the name of your institution and the path to your university's logo in **index.Rmd**:

```
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 and 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
```



Title of your Thesis

John Doe

Thesis committee

Promotor:
Prof.dr J. Smith
Professor of Geo-information Science and Remote Sensing
Wageningen University

Co-promotors:
Dr. Name of co-promotor
Assistant Professor, Laboratory of Geo-information Science and Remote Sensing
Wageningen University

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

This research was conducted under the auspices of the C.T. de Wit Graduate School of Production Ecology & Resource Conservation (PE&RC)

Title of your thesis

John Doe

Thesis
submitted in fulfilment 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.

John Doe
Title of your thesis
77 pages.

PhD thesis, Wageningen University, Wageningen, NL (2015)
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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 praises 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.

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 Yihui Xie for creating `knitr` which introduced R Markdown as a way of embedding code in Markdown documents, and `bookdown` which added tools for technical and longer-form writing.

Special thanks to Chester Ismay, who created the `thesisdown` package that helped many a PhD student write their theses in R Markdown. And a very special thanks to John McManigle, whose adaption of Sam Evans' adaptation of Keith Gillow's original maths template for writing an Oxford University DPhil thesis in LaTeX provided the template that I in turn adapted for R Markdown.

Finally, profuse thanks to JJ Allaire, the founder and CEO of RStudio, and Hadley Wickham, the mastermind of the tidyverse 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.

Ulrik Lyngs
Linacre College, Oxford
2 December 2018

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

```
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

A list of PDBs was assembled that represented either a representative sample of a variety of proteins, with a resolution better than 3A, (HEM and HEC) or, all proteins containing these ligands were downloaded from the PDB (in the case of SRM, VER, VEA). Not all downloaded PDBs were appropriate for this study (e.g. contained "wobble" structures) and therefore the amount of PDBs was culled. The datasets are current as of 16 August 2021.

The size of the datasets actually used in the study were as follows: HEM

(n=58), HEC(n=14), SRM (n=9), VER (n=2) and VEA (n=2) for a combined n=4 for VERDOHEME.

The name of all proteins used in the study and their source organism are provided tables within Appendix B.1.

7.2 Preprocessing

Many of the PDBs downloaded were multimeric structures. While many of the scripts employed in the study may function with multimeric structures, the number of subunits per protein (FIXME! better way to say this?) would skew results in favor of multimeric proteins with more subunits. The information gleaned from similar subunits would also not be of utility in this study.

Therefore all downloaded PDBs were converted to monomeric structures. This was achieved by saving a single chain (chain A) of each PDB and eliminating all other chains. The single chain was then saved as a PDB and used in all subsequent scripts.

7.3 Processing Monomers

UCSF-Chimera was used to generate all data in this study. Multiple scripts were employed to achieve a high-throughput process where all monomeric PDBs could be processed in the same session.

Chimera was used to predict the following qualities: Volume of the ligand binding pocket, accessible and excluded surface area of the ligand, and accessible and excluded surface area of the binding pocket. These calculations require a population of atoms to be selected for the calculation.

Atoms were selected within a distance cutoff, to be considered as "interacting" with the ligand or forming the binding pocket. Distance cutoffs from the ligand of 5A and 7A were chosen; for the predicted qualities, the algorithms were run twice to get values at 5A and 7A. For the distance and angle calculations, only the 7A distance cutoff was used, as the cutoff does not factor into any calculations and may be set during analysis.

as these are selected arbitrarily, data from the 5A and 7A runs are overlaid in the figures reported in Appendix **??**. Data tables are also provided in Appendix **??**.

7.3.1 Amino Acid Frequency

Amino acids within the bounds of the lower and upper distance cutoff were selected and recorded. These were then counted for frequency per residue.

7.3.2 Volume Calculations

Volume of the binding pocket was predicted via Surfnet, run with default parameters of Grid Interval = 1.0 and Distance Cutoff = 10.0 (the latter option does not relate to the distance cutoff from the ligand(FIXME! find source for this, appears 100% to be true?)).

7.3.3 Surface Area Calculations

Excluded and accessible surface areas of both the ligand and the binding pocket were calcualted using Chimera's "surf" algorithm, available as "Measure Volume and Area" via the GUI.

7.3.4 Distance Calculations

Distances of amino acids from the ligand could not be calculated accurately nor precisely in a direct way. Instead, distances for each atom composing a residue were calculated. The distances of all atoms within a residue were averaged, and this value was taken as the mean distance of the entire residue and used in subsequent steps.

The data produced in this step therefore include the mean distance of each amino acid. This is traceable, and the angular data below are cross-referenced with this list of distances. All data shown in figures (FIME! Also for tables?) are multidimensional and may be filtered for distance.

7.3.5 Planar Angle Calculations

Individual residues and the ligand were defined as axes The angle between each residue's axis and the axis of the ligand were calculated. Each axis functions essentially as a separate plane. (FIXME! Include a picture of what this looks like?) This employed the "define axis", and "angle" functions of Chimera; the Axes/Planes/Centroids Structural Analysis function of Chimera via GUI.

7.3.6 CA-CB-Fe Calculations

Residues within the distance cutoff were examined one by one. The angle of between each residue's carbon alpha (CA) and carbon beta (CB) and the Fe of the ligand was calculated, using the "angle" function of Chimera. The ligand nor the Fe atom were compared with themselves.

7.4 Import to R

All data were imported to R and processed from text files into organized data formats. R was used to cross-reference angle and distance data. All plots and tables were constructed using R and imported directly to this document using Rmarkdown.

8
Results

Data are reported as figures in Appendix **??** and tables in Appendix **??**. Data are organized by result e.g. Volume, and then by ligand.

9 Discussion

This section is organized by type of result; figures and tables referenced are within the appendices.

9.1 AA Frequency Discussion

Amino acid frequencies within the 5A and 7A distance cutoffs of the ligand reported in Appendix **??** and (FIXME! Missing amino acid tables. For HEM and HEC, nonpolar amino acids are the most frequent. This may indicate that nonpolar amino acids are extremely important to stabilizing the binding pocket.

For SRM, this is not the case. HEM and HEC are very similar, but SRM is quite different. For SRM we find that arginine is extremely frequent to find in the pocket (amongst n=9). This is perhaps expected given the exposure of charged groups on SRM, but the degree of the effect is very notable. Glycine and Lysine and other small residues are also highly present. Perhaps this indicates a selection for small residues in the binding pocket to accomodate SRM.

Verdoheme, again, has a very small sample size (n=4). But the results appear to follow trends seen in other ligands; a preference for nonpolar, charged, or small residues. Leucine is the most preferred of these, along with alanine - two small nonpolar amino acids. These results, although limited, reinforce the trend of

an especially important composition of amino acids in the binding pocket rather than the coordinating amino acids.

9.2 Volume Discussion

Besides HEM, much of the volume data for the different ligands did not closely agree between different distance cutoffs. Most of the data did however fall within reasonable bounds, regardless of distance cutoffs.

HEM appears to require a pocket volume of between 800 and 1200 A^3. Data reported for this quality range between 500 and 2000 A^3. These outliers can perhaps be explained by proteins with exceptionally large binding pockets, but are more likely an indication of the imperfections in the volume calculation algorithm, highlighting the need for studies that take into account a multiplicity of PDBs to evaluate the size of a binding pocket.

HEC volume data centers around 800-1100A^3. This molecule is very similar to HEM and these results are somewhat expected. Outliers again can perhaps be explained by the volume calculation algorithm.

SRM and Verdoheme suffer from a low number of sample data. SRM appears to center at 1000-1200 A^3, again somewhat confirmed by other ligands examined in the study.

But Verdoheme has a near equal distribution of samples from 700-1450 A^3; this lack of agreement precludes a range that may be suspected to be the "real" volume.

9.3 Ligand Solvent Excluded Surface Area Discussion

The limitations of the limited sample size can be seen in this quality as well.

HEM appears to have a ligand surface area of approximately 500-700 A^2. HEC follows a similar trend.

However, for SRM and Verdoheme, data are more scattered. Trends cannot be derived from these data.

9.4 Ligand Solvent Accessible Surface Area Discussion

HEM has a strong agreement of data at approximately 1000-1250 A^2. HEC, slightly more scattered, appears to agree from 750-1250 A^2.

SRM, despite its limited sample size, has strong agreement for this quality: it ranges from about 1000-1050 A^2.

VERDOHEME is highly scattered for this measure. Verdoheme ranges from 750-1800 A^2.

9.5 Pocket Solvent Excluded Surface Area

HEM data has poor agreement for this measure. Data is concentrated from 5000-15000 A^2, but this is a very large range and not very useful.

HEC agrees in a somewhat tighter range: most data fall within 5000-7500 A^2; still not very useful but better than HEM.

Most SRM data fall within 21000-22000 A^2.

Verdoheme data range from 9200 to 10000 A^2.

For this measure, then, we find that SRM and Verdoheme have a fairly specific range of predicted solvent excluded surface area for their binding pockets.

9.6 Pocket Solvent Accessible Surface Area

The results for this measure follow the trends for the previous section.

Most HEM data fall from 5000-15000 A^2. HEC data mostly fall from 5000-7500 A^2.

SRM data is highly concentrated at approximately 21000 A^2, more specific than the pocket solvent excluded surface area.

Verdoheme data range from 10000-11000 A^2.

9.7 All Planar Angles

These data, for all ligands, largely serve to compare as noise for the next section. The planar angles of all residues falling within the upper distance cutoff are plotted.

A notable exception is HEC; the plot for this ligand seems to suggest that GLU and LYS have fairly specific planar angles with the ligand. (FIXME! Check out the distance tables to drill down further)

9.8 Planar Angles of Closest Residues

Here, the three closest residues to the ligand in each PDDB and their planar angle to the ligand are plotted.

HEM has a fairly inconclusive set of data for this measure. GLU and GLN nearby HEM do appear to fall within a tight range, though, of approximately 75 degrees and 80 degrees respectively.

The data for residues nearby HEC diverge from what is found for all residues around HEC. The most agreement is found for ILE and LYS, with angles concentrated about 50 degrees and 75 degrees, respectively.

Only three types of residues appear nearby SRM: CYS, LYS, and ARG. Although their angles vary wildly, these data suggest these residues are important to the coordination fo SRM. (FIXME! Add reasoning)

Verdoheme also has a small selection of residues that are close to the ligand. GLY and HIS are the only residues that are close to the ligand in the PDBs used in this study. (FIXME! Add reasoning... or qualifier statement n=2)

9.9 All CA-CB-Fe Angles

All residues have a broad range of angles in relation to HEM.

Most residues have a broad range of angles for HEC, with the exception of THR, which has a tight distribution around 100 degrees. This result only appears

here and does not follow for the closest residues, and therefore may be due to a small sample size of THR residues.

SRM appears to have tight distributions of angles when considering all residues; the residues closest to SRM do not echo this. Although likely attributable to a small sample size, there appear several residues with specific angles: ALA around 50 degrees, GLN around 140-150 degrees, and SER around 50 degrees.

Verdoheme... (FIXME! Confer with JeanDi before we report more of these angles. Not sure I'm going about it in an informative way. Also add figure numbers.)

9.10 CA-CB-Fe Angles of Closest Residues

Most notably, HIS is the only residue that appears closeby Verdoheme, and falls within a range of 106-116 degrees.

10
Limitations of the Study

Limited sample size

Limited experimental data to reference to verify

NO experimental data in this study to verify, all theoretical

Only one software package/few algorithms used to calculate all these properties. Ot

Algorithms may introduce bias based on how they work e.g. all the bubbles

Arbitrary selection of parameters; some based on rule of thumb or visual evaluation

Unknown if the qualities measured are truly the most critical for the heme binding.

Visual examination itself to OK the parameters/algorithms can introduce bias

11 Conclusion

Multiple qualities were predicted and data gathered from representative or whole population (FIXME! better way to put this?) datasets of ligands for hemoproteins. Some qualities per ligand follow very tight distributions and suggest a requirement for ligand binding, e.g. specific volume of binding pockets.

This is not the case for all qualities. Surface areas and angles of residues in relation to the ligands appear to diverge greately. This suggests the binding pockets, while having some useful trends (e.g. high populations of nonpolar amino acids), may still be highly variable. The results of this study are limited by the small sample size, but suggest that binding pockets for hemoproteins have some requirements for binding that may be overlooked, e.g. a high population of nonpolar amino acids. These results may be useful in the design of hemoproteins in the future, in combination with other approaches, to at least narrow down screening efforts and determine realistic designs and modifications.

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

A
Figures

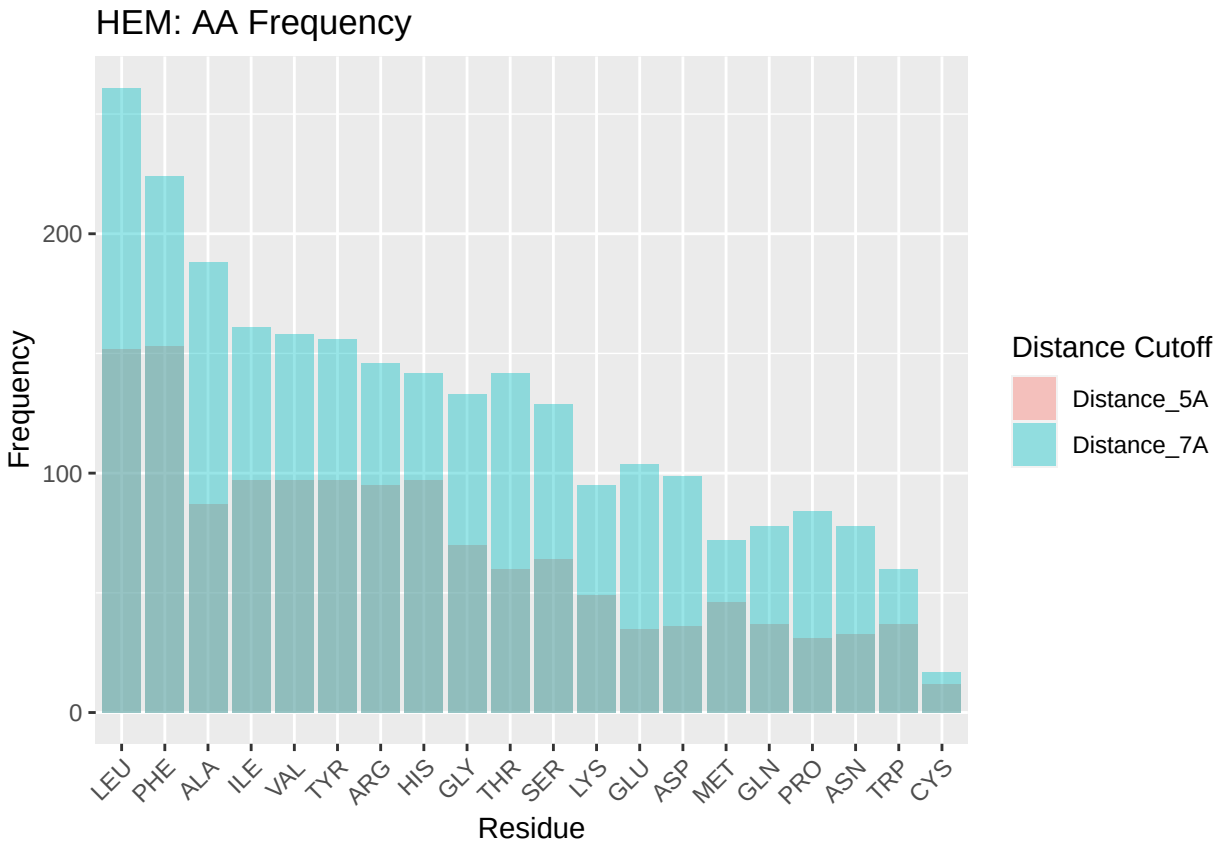

Figure A.1: HEM: AA Frequency

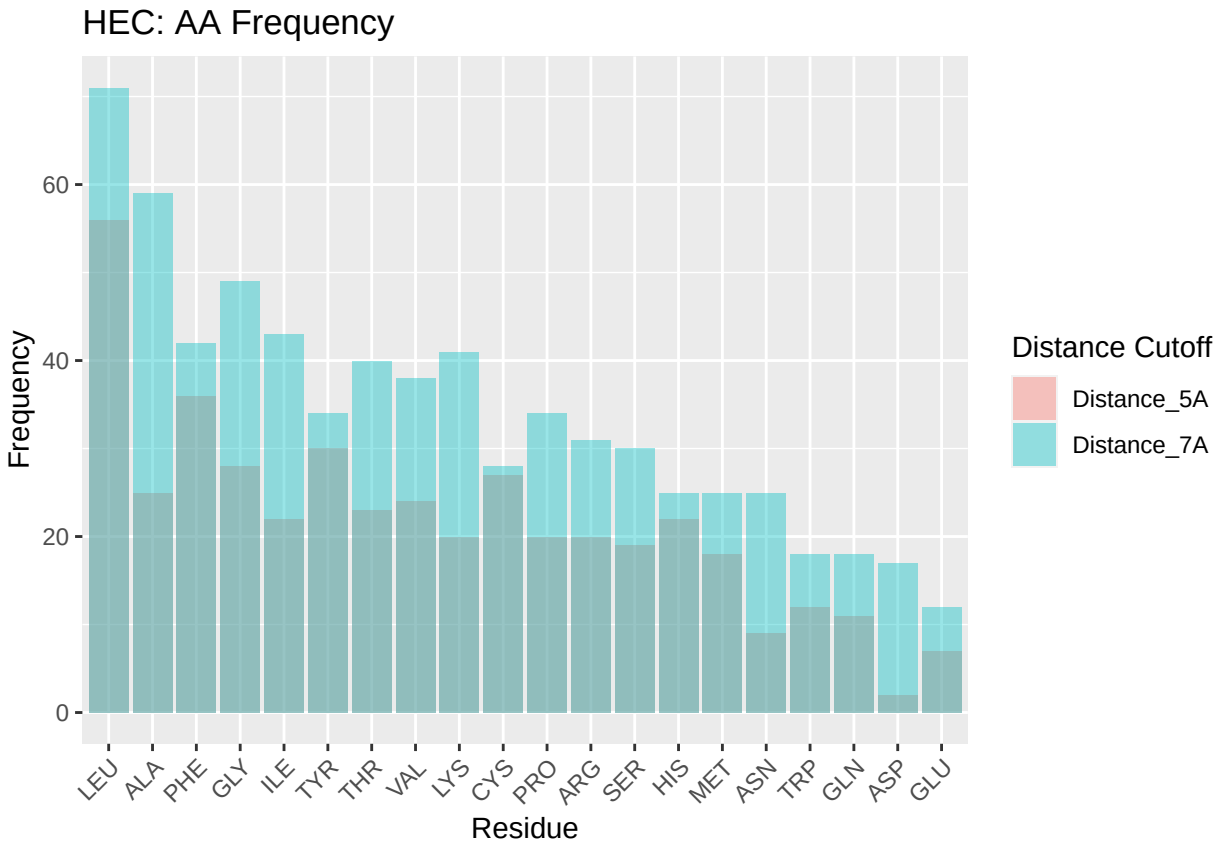

Figure A.2: HEC: AA Frequency

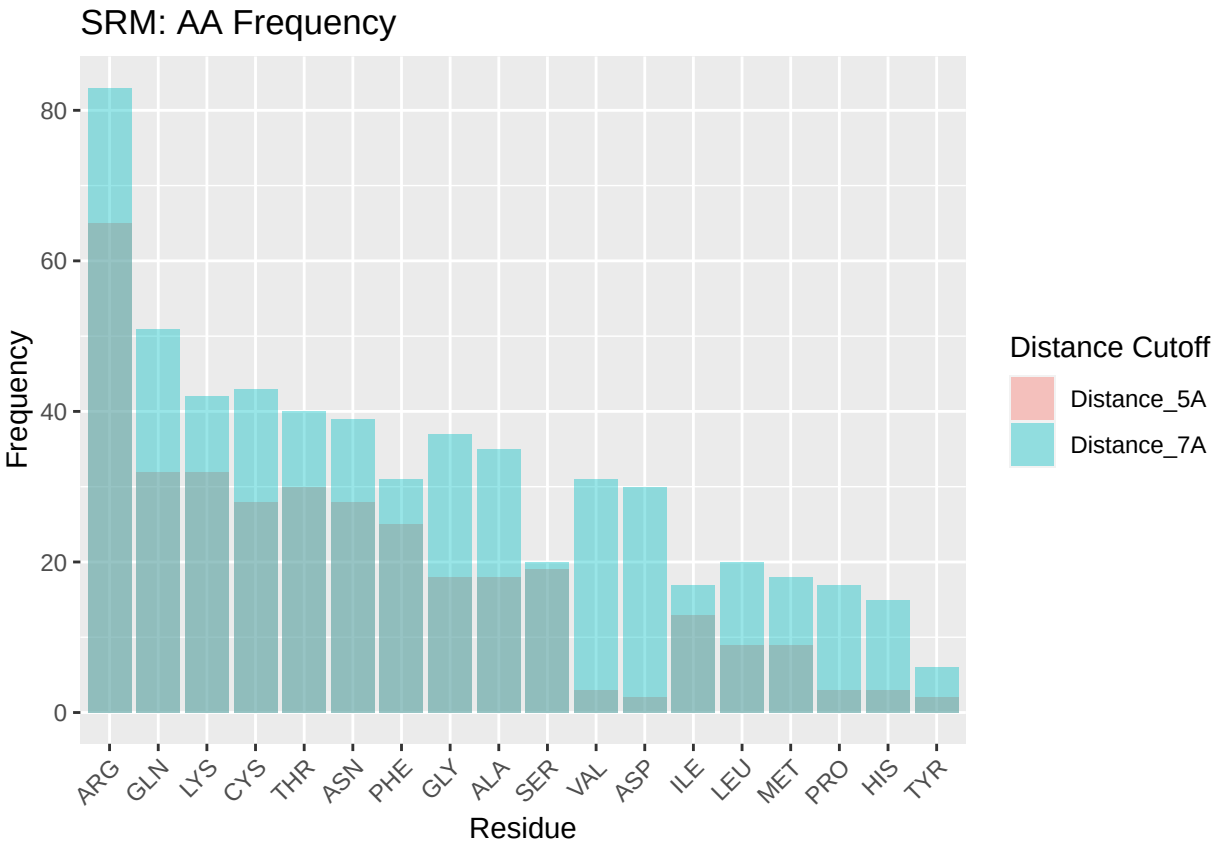

Figure A.3: SRM: AA Frequency

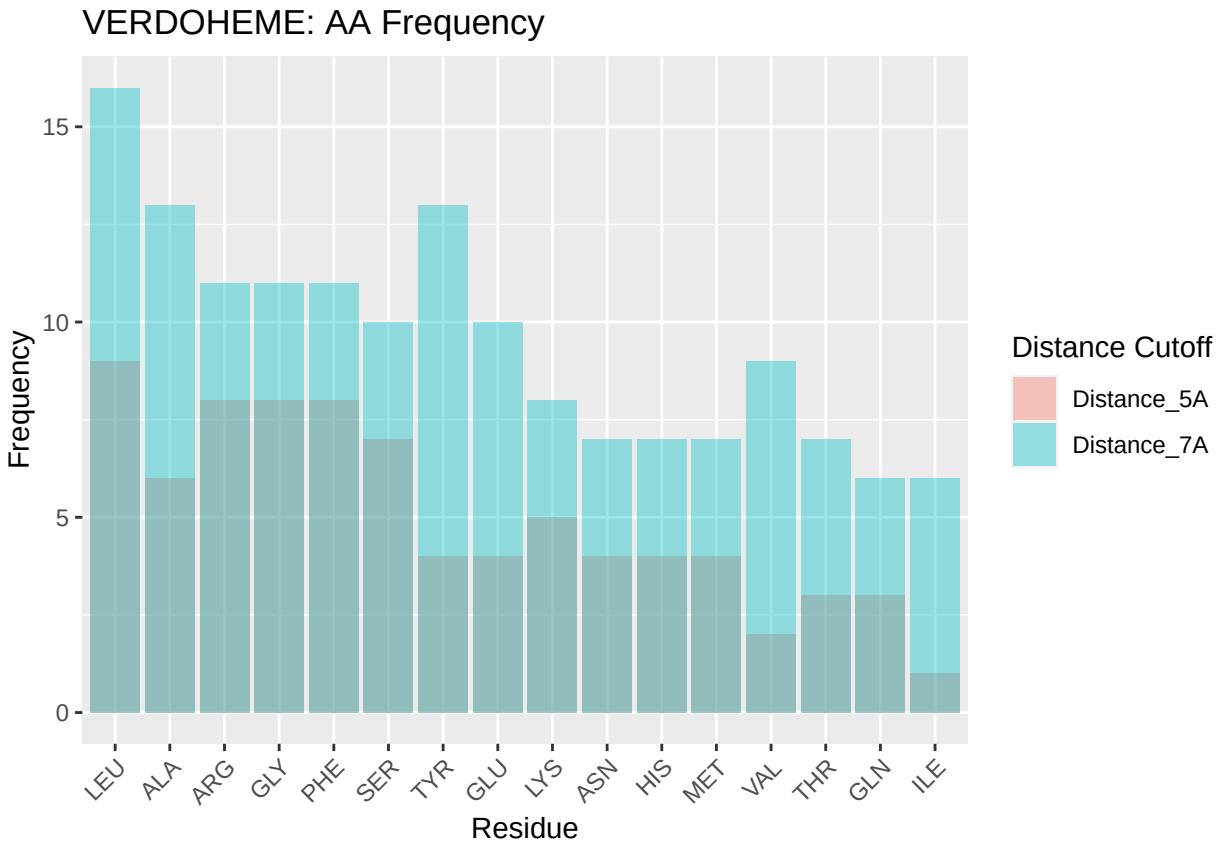

Figure A.4: VERDOHEME: AA Frequency

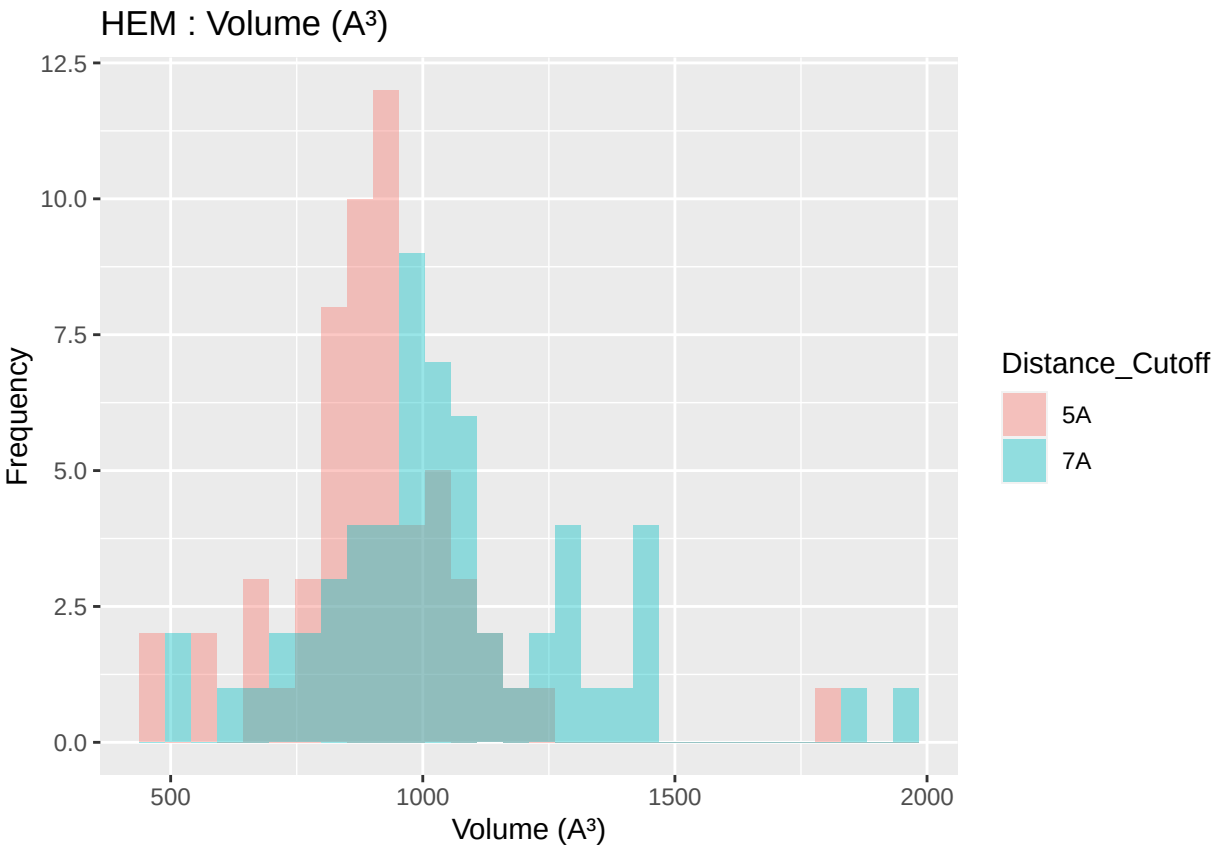

Figure A.5: HEM: Volume

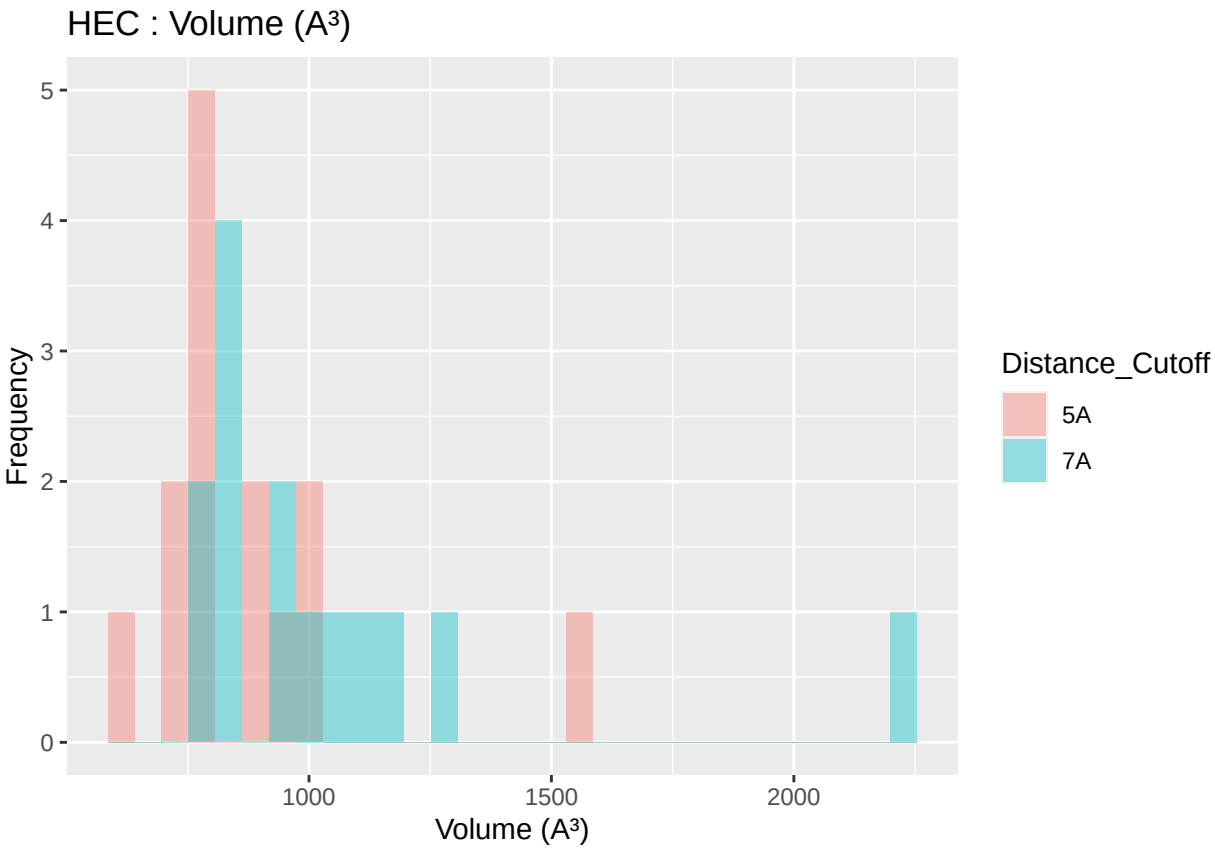

Figure A.6: HEC: Volume

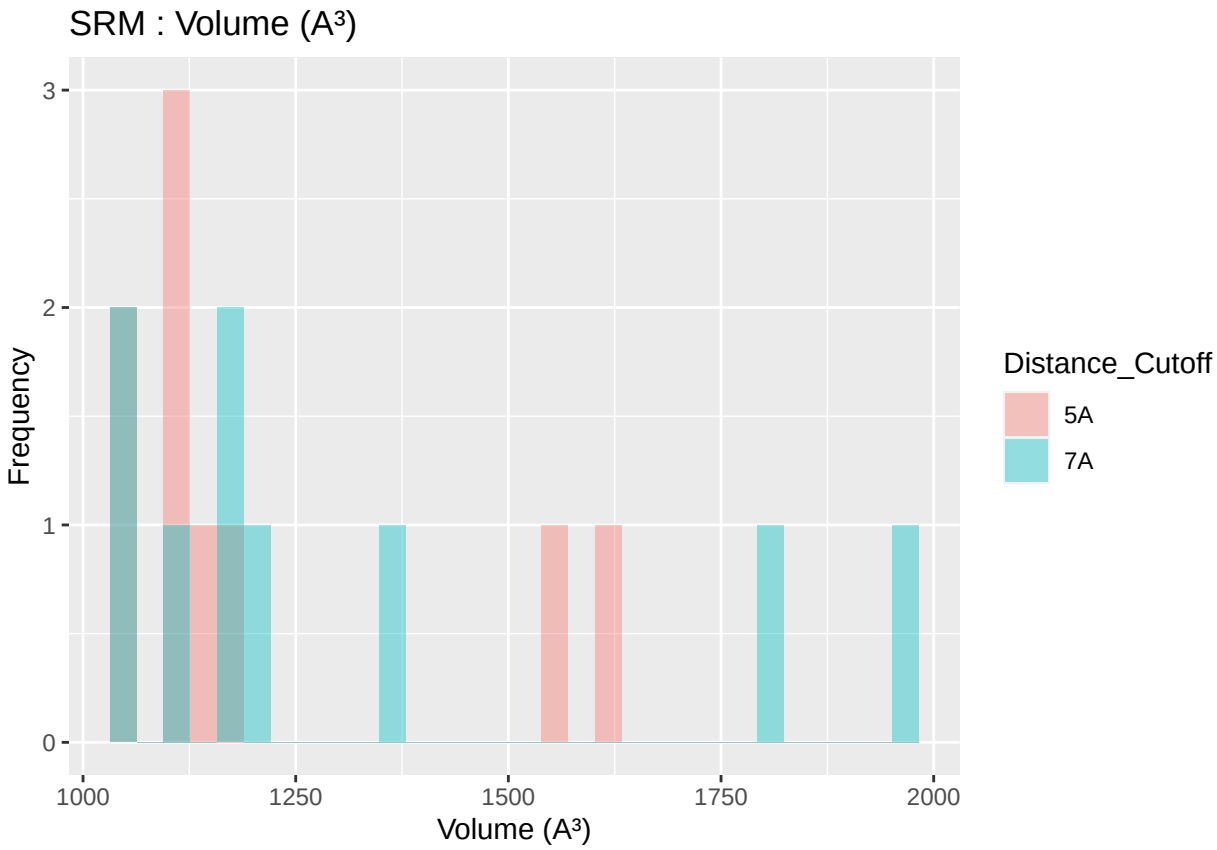

Figure A.7: SRM: Volume

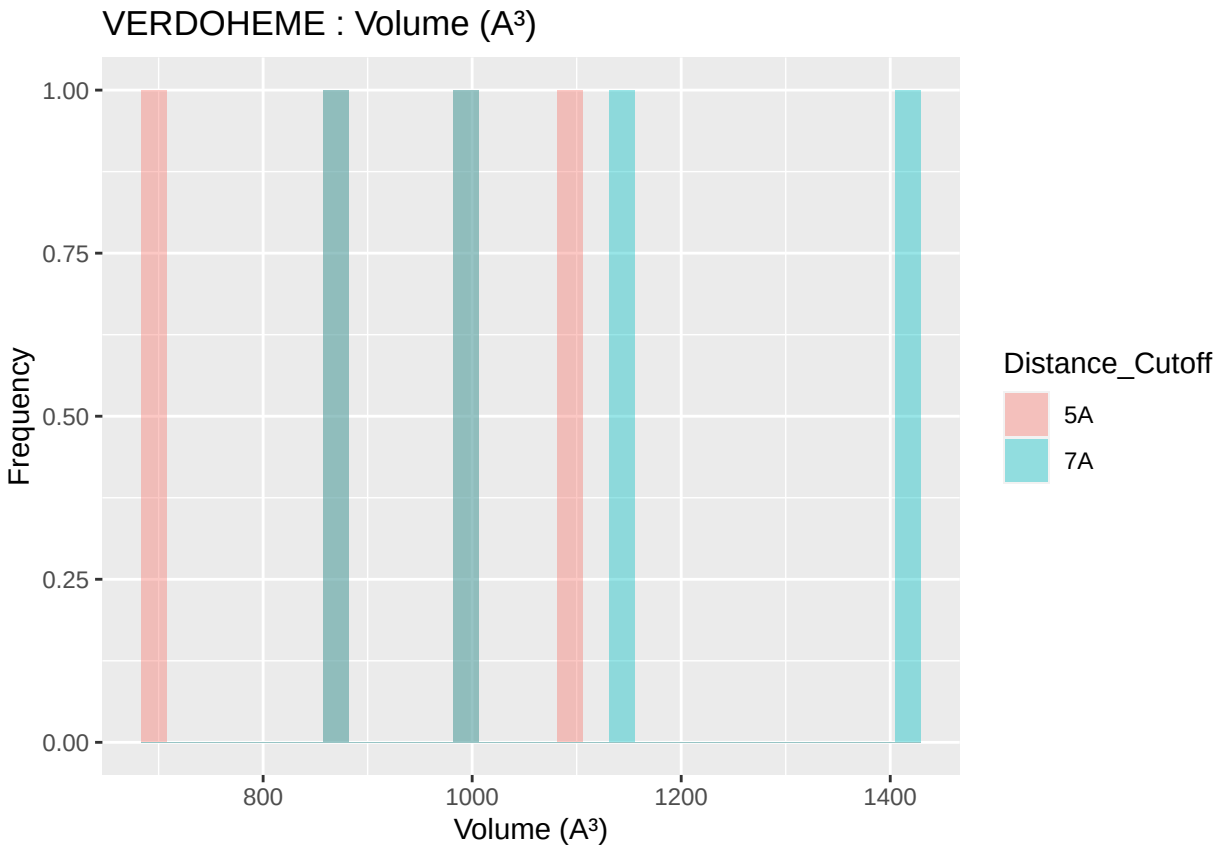

Figure A.8: VERDOHEME: Volume

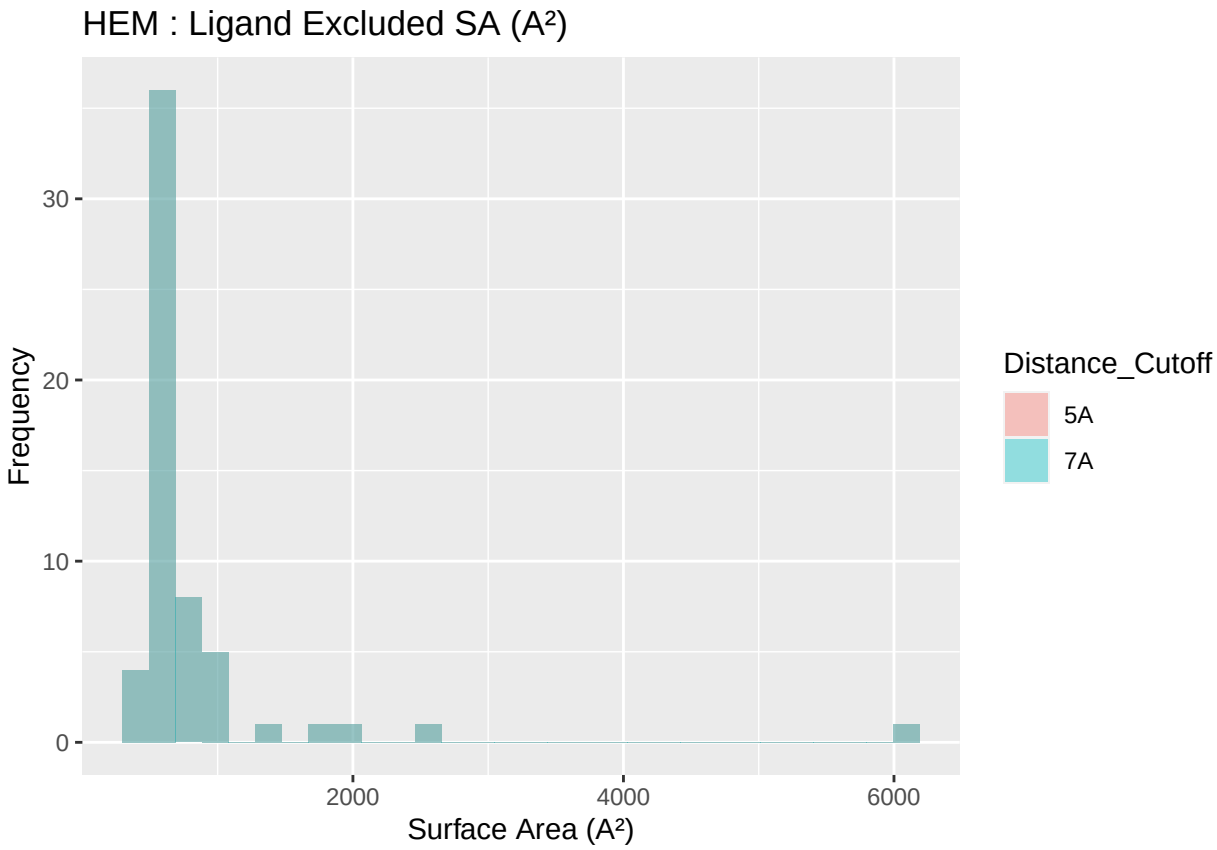

Figure A.9: HEM: Ligand Excluded Suface Area

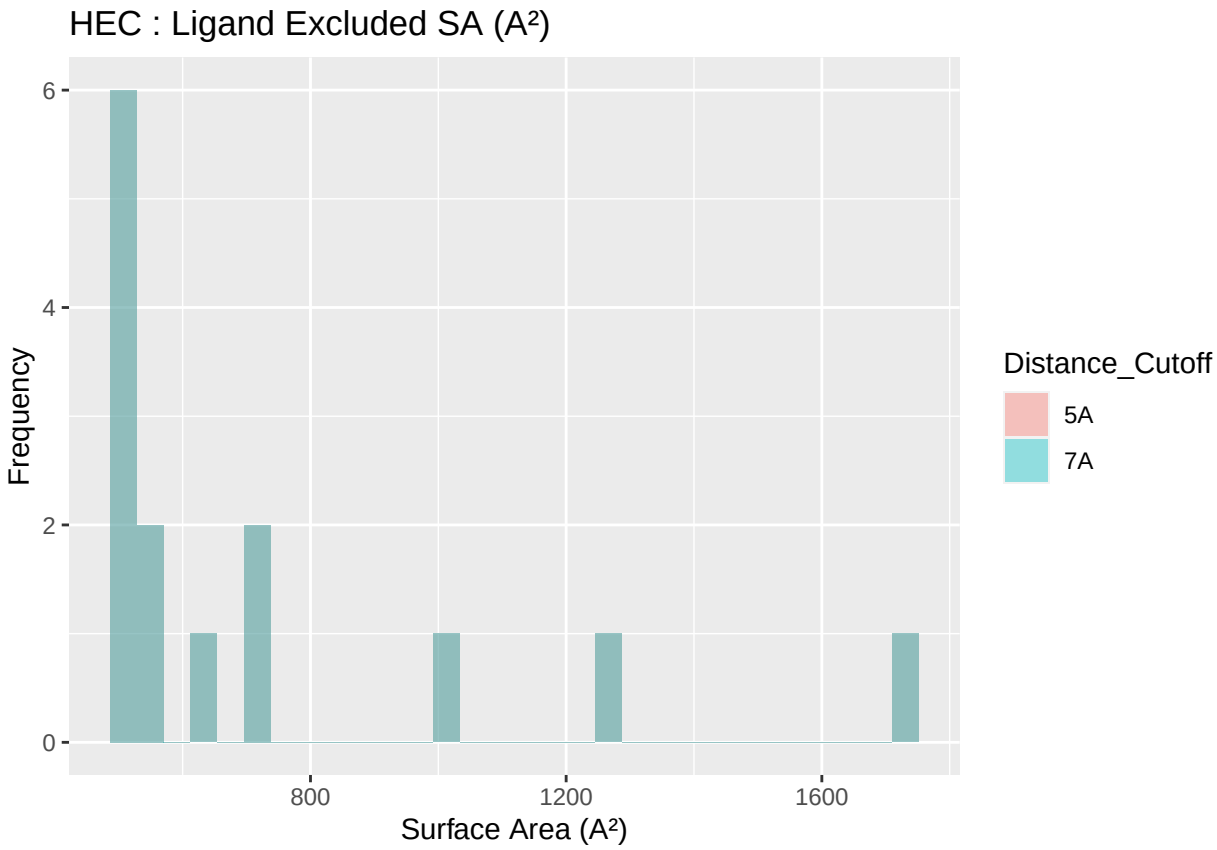

Figure A.10: HEC: Ligand Excluded Suface Area

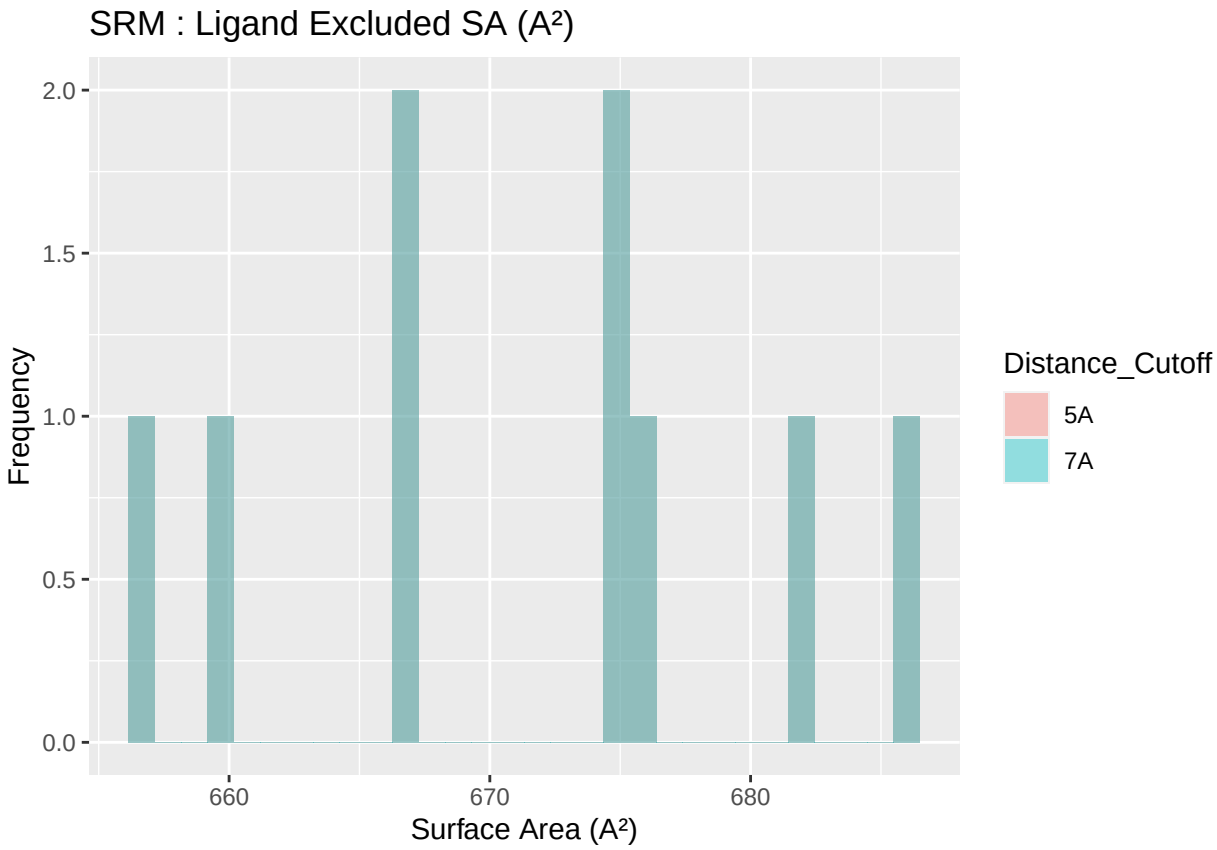

Figure A.11: SRM: Ligand Excluded Suface Area

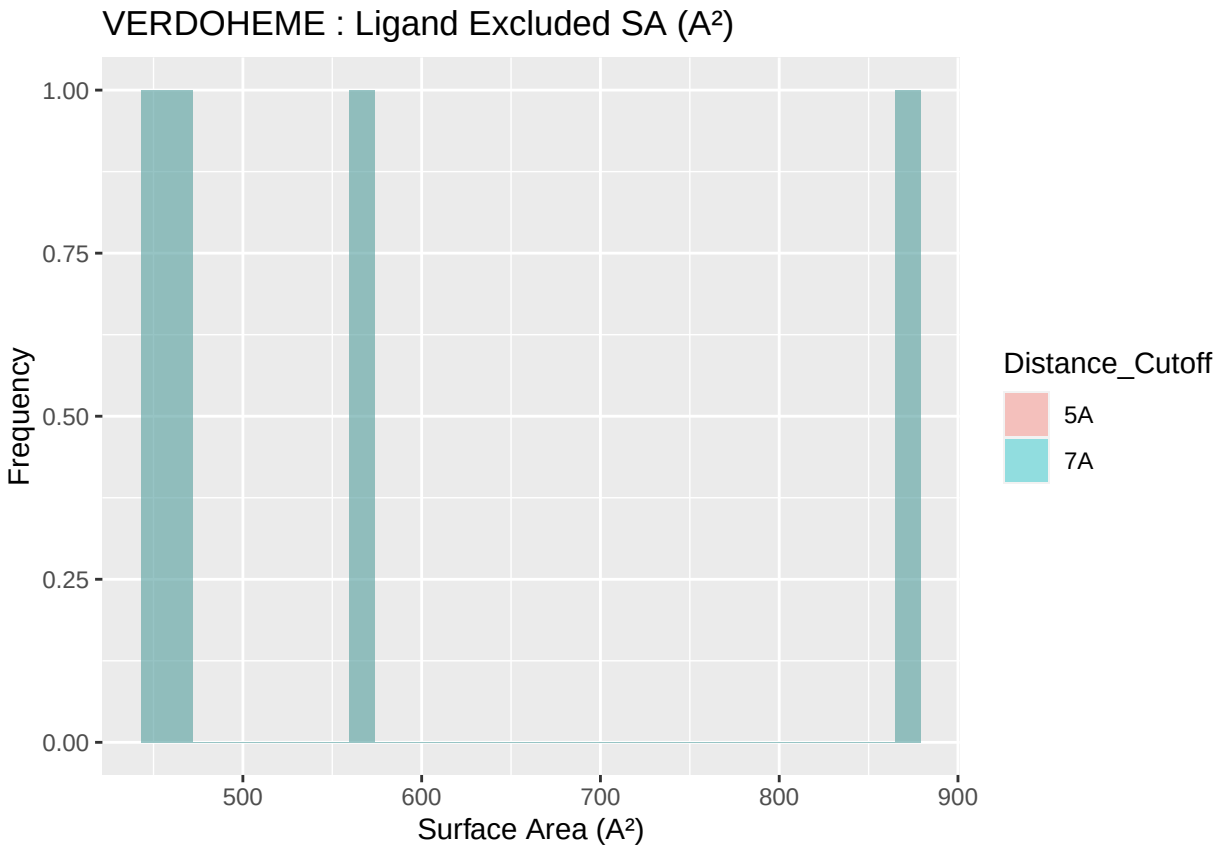

Figure A.12: VERDOHEME: Ligand Excluded Suface Area

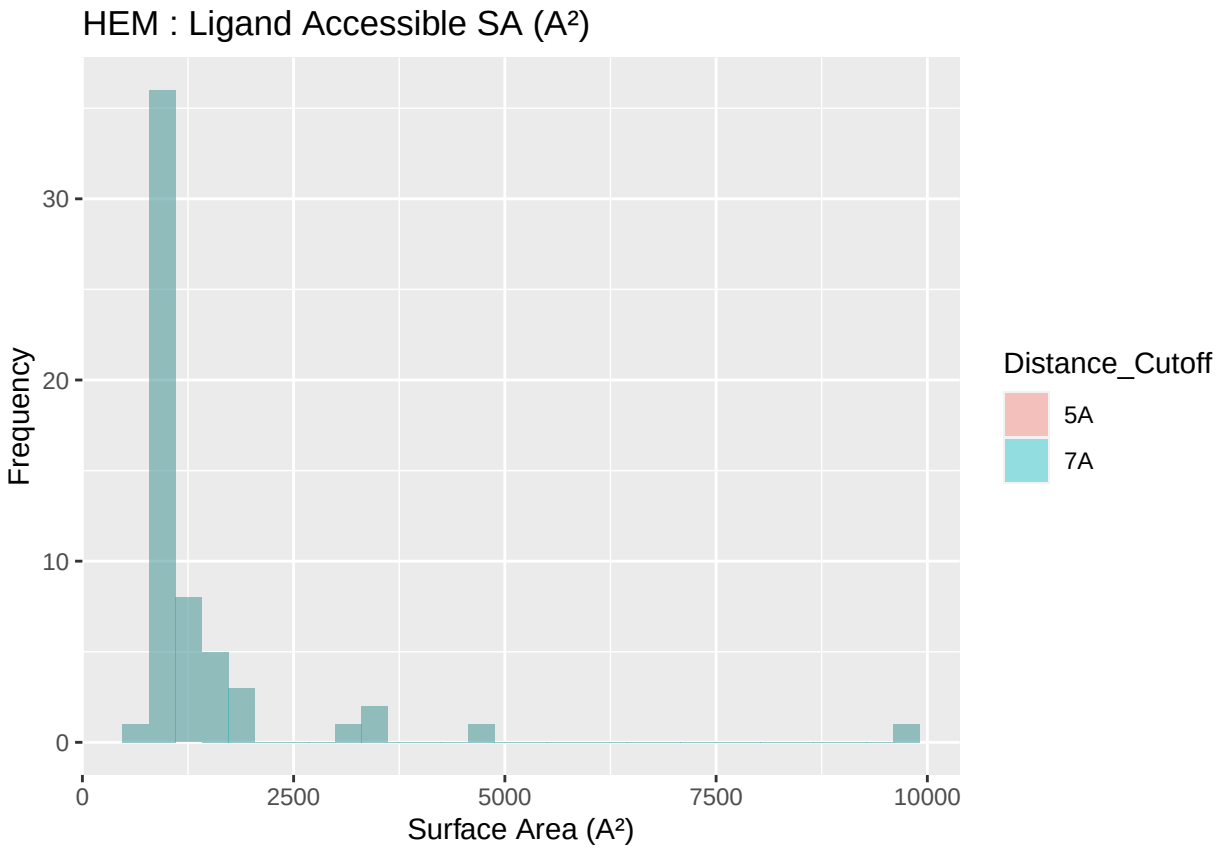

Figure A.13: HEM: Ligand Accessible Surface Area

Figure A.14: HEC: Ligand Accessible Surface Area

Figure A.15: SRM: Ligand Accessible Surface Area

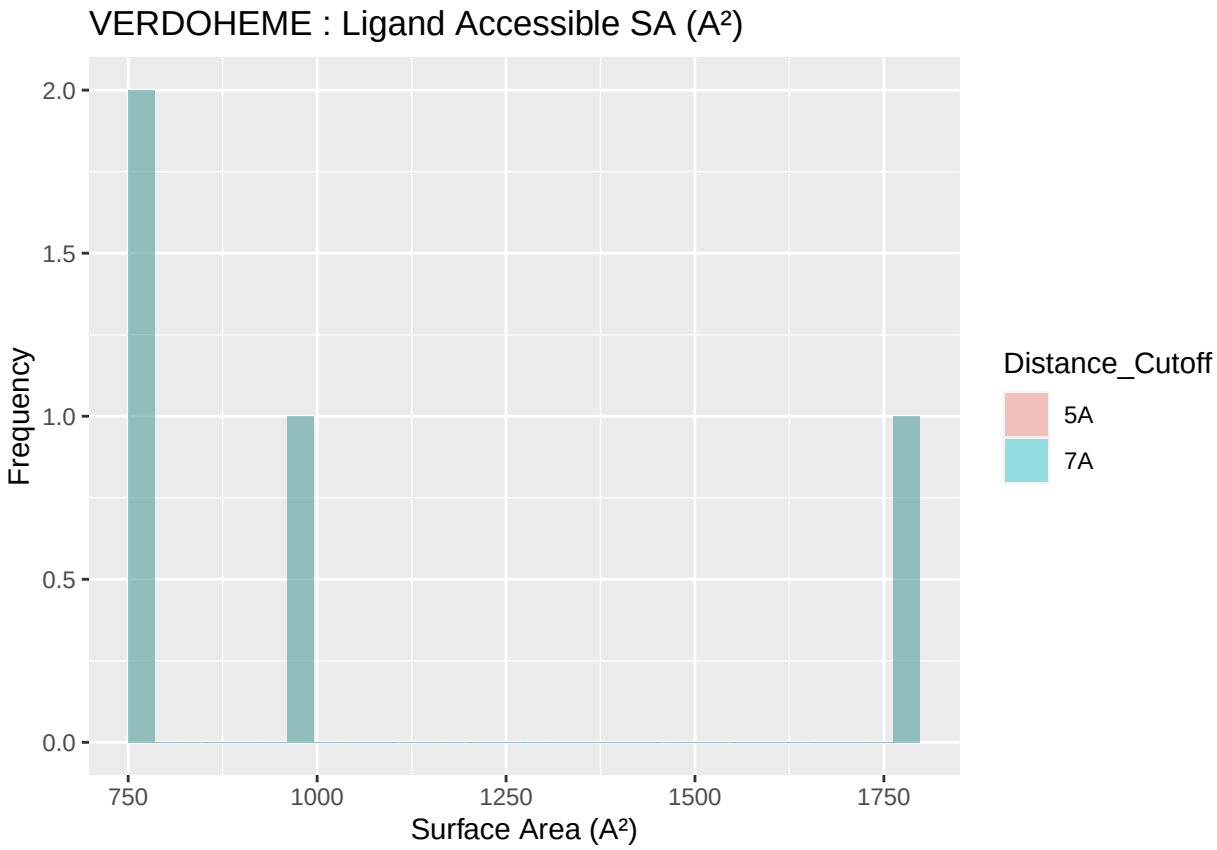

Figure A.16: VERDOHEME: Ligand Accessible Surface Area

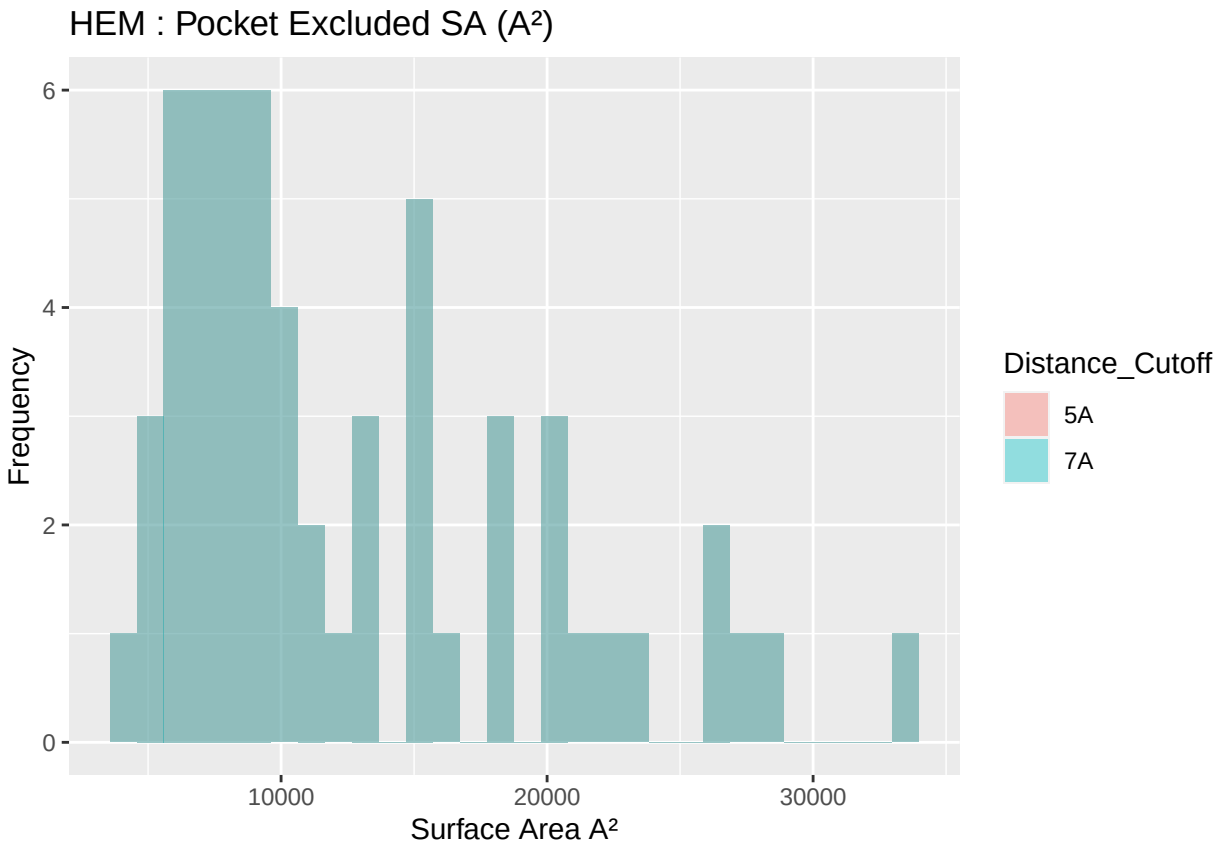

Figure A.17: HEM: Pocket Excluded Surface Area

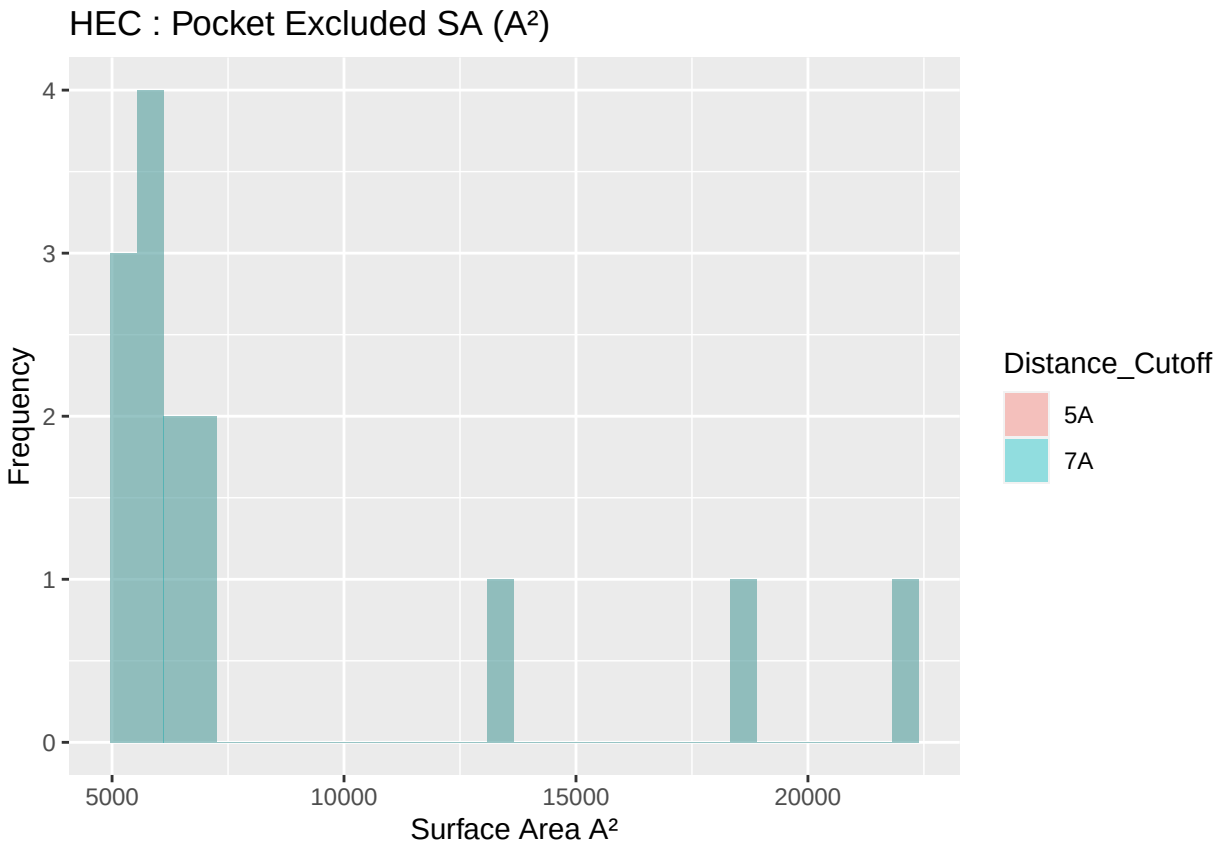

Figure A.18: HEC: Pocket Excluded Surface Area

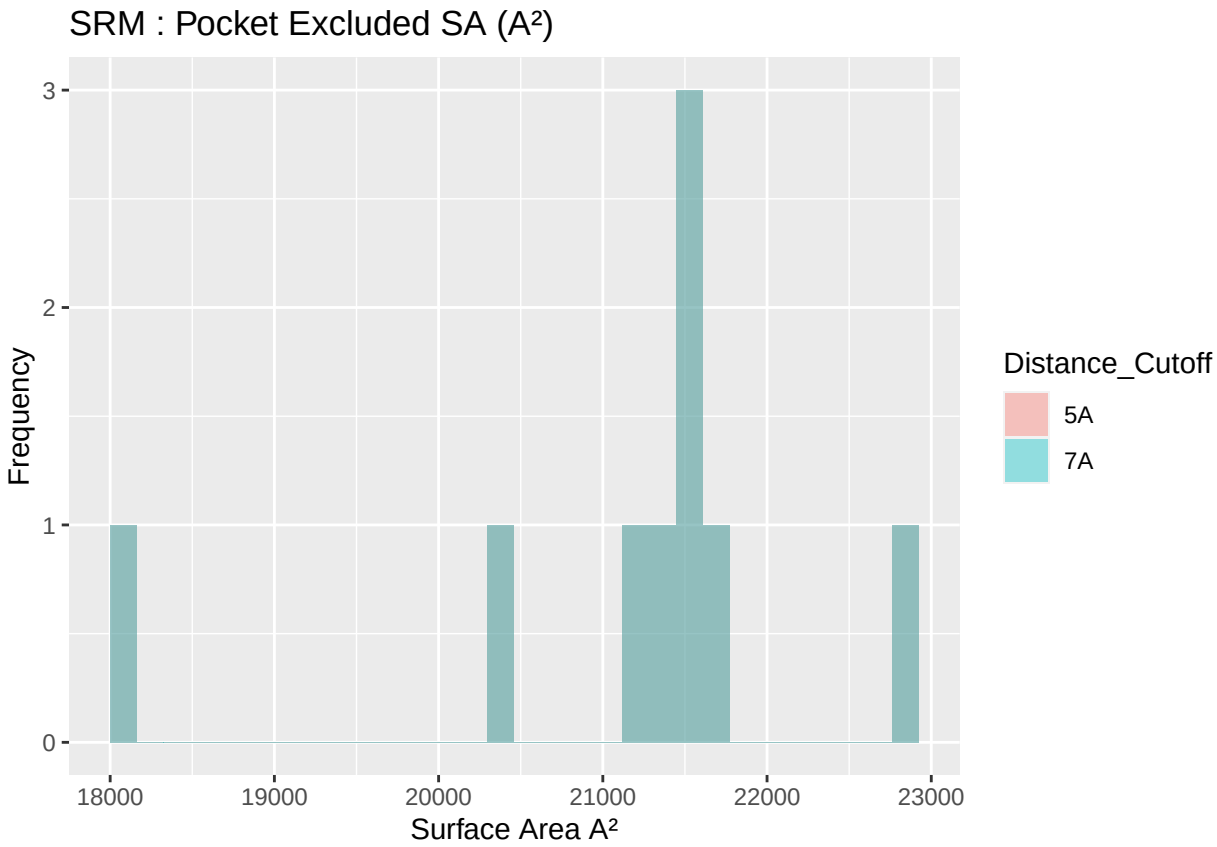

Figure A.19: SRM: Pocket Excluded Surface Area

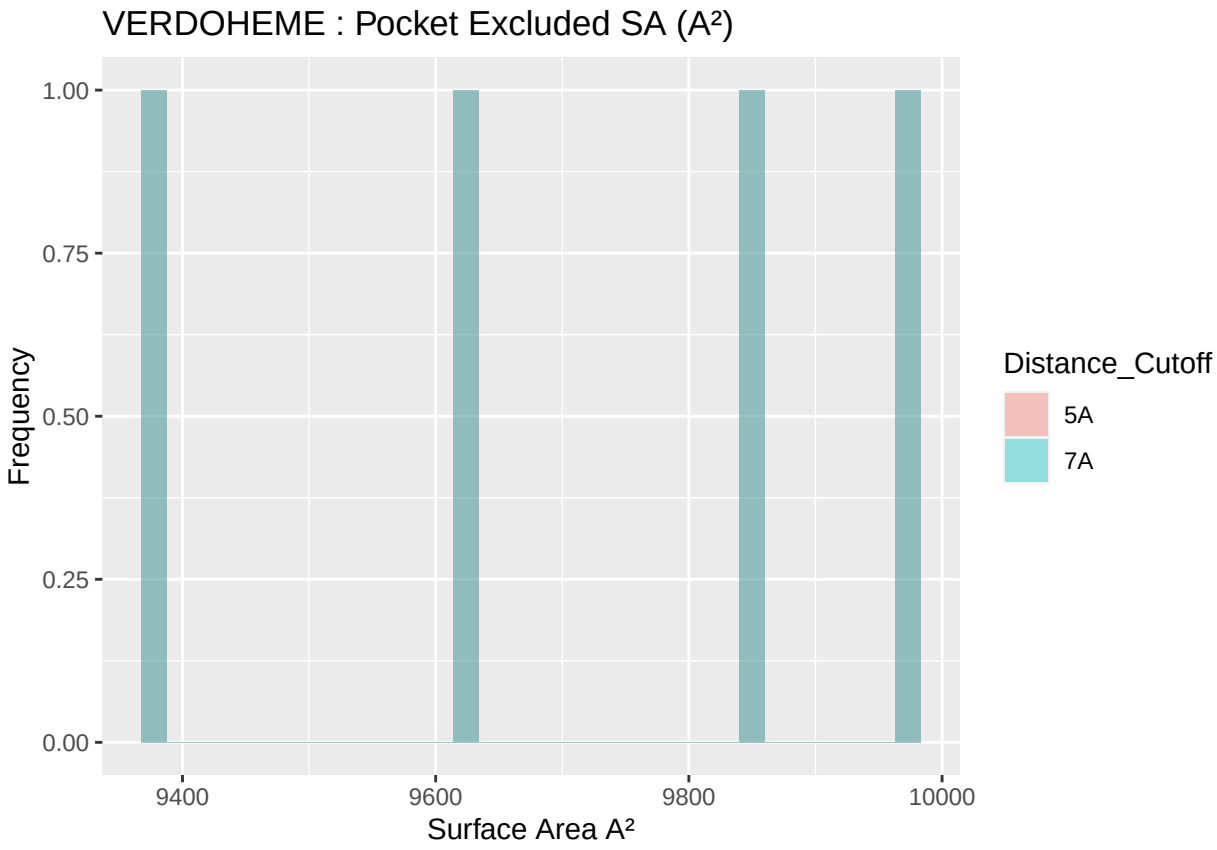

Figure A.20: VERDOHEME: Pocket Excluded Surface Area

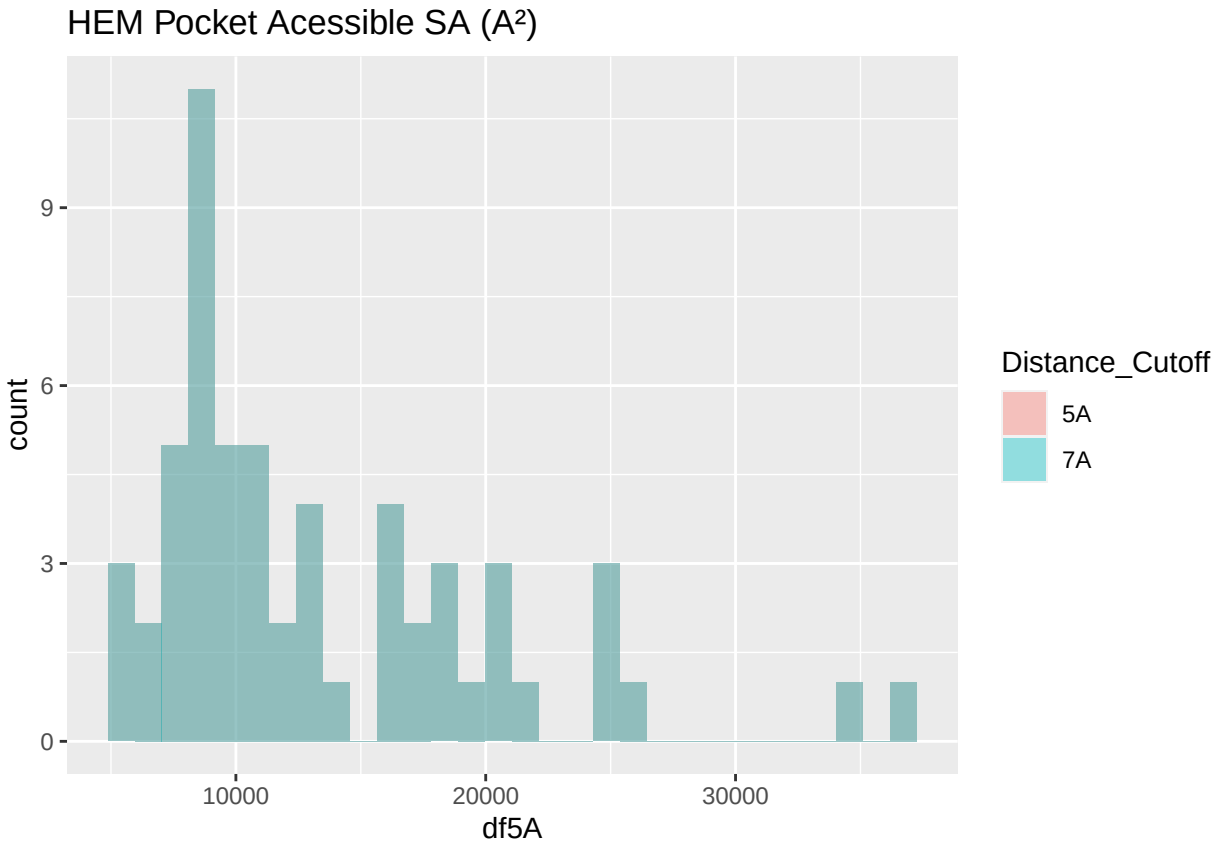

Figure A.21: HEM: Pocket Accessible Surface Area

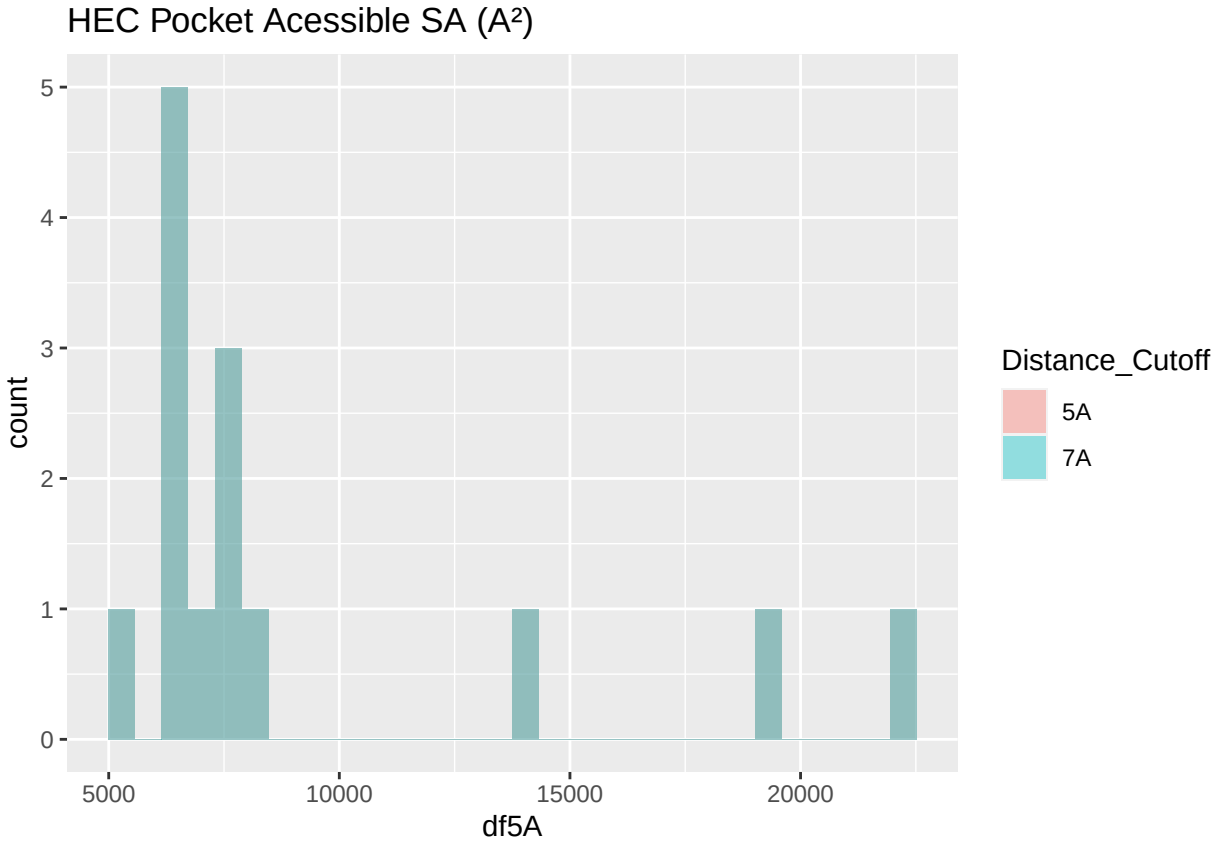

Figure A.22: HEC: Pocket Accessible Surface Area

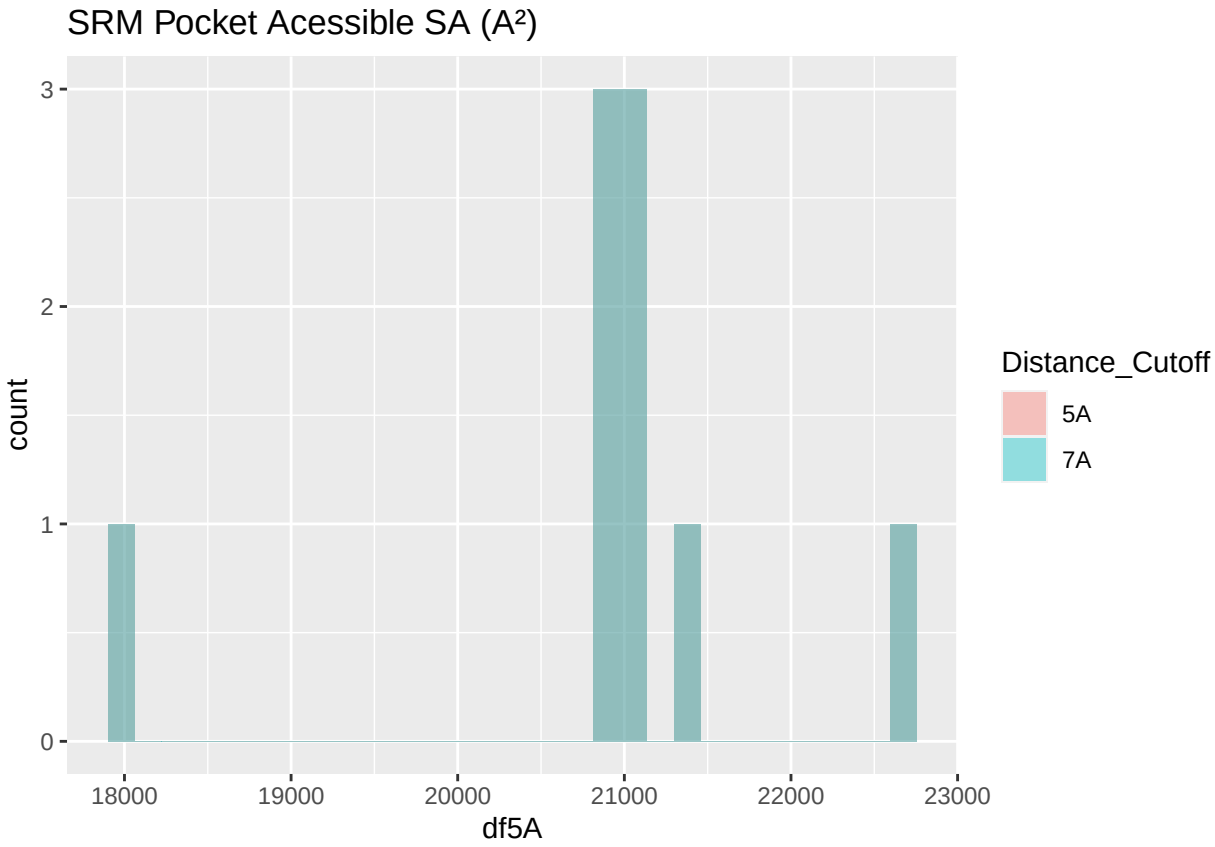

Figure A.23: SRM: Pocket Accessible Surface Area

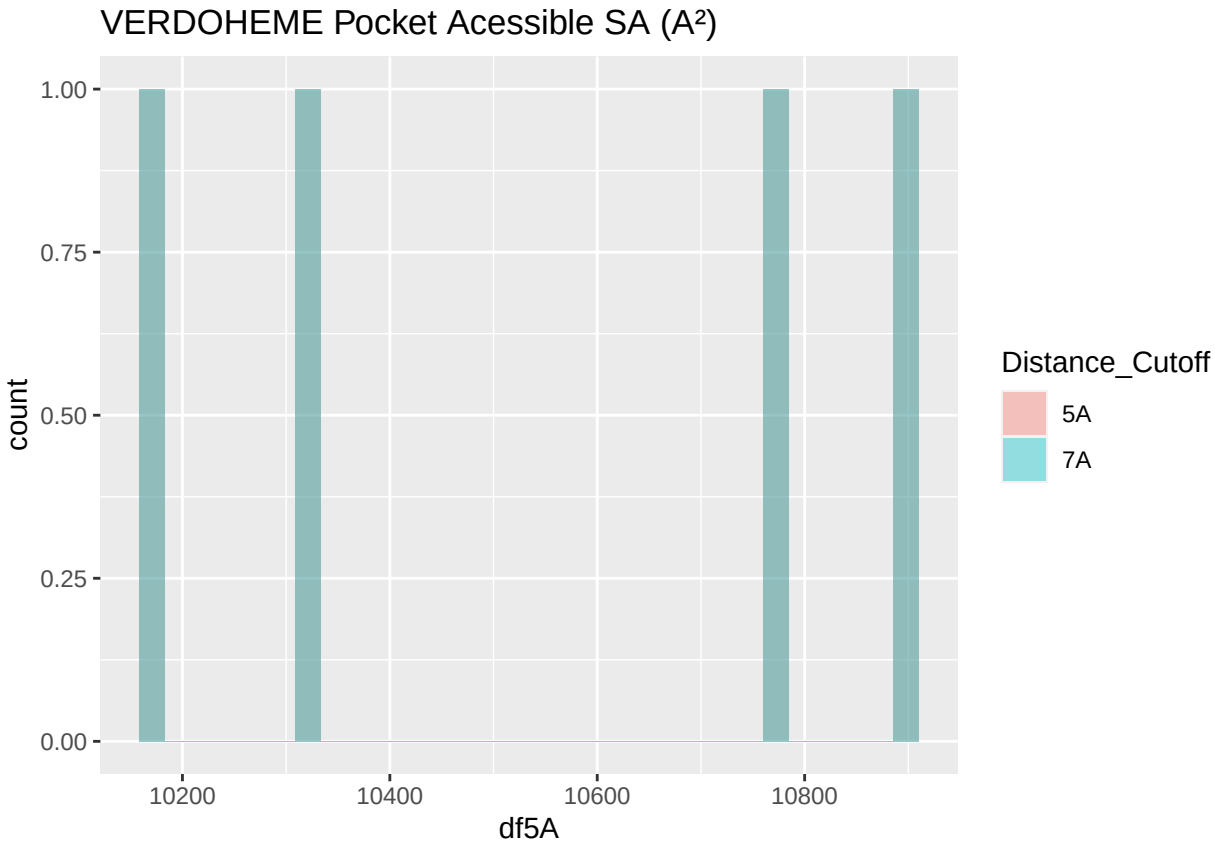

Figure A.24: VERDOHEME: Pocket Accessible Surface Area

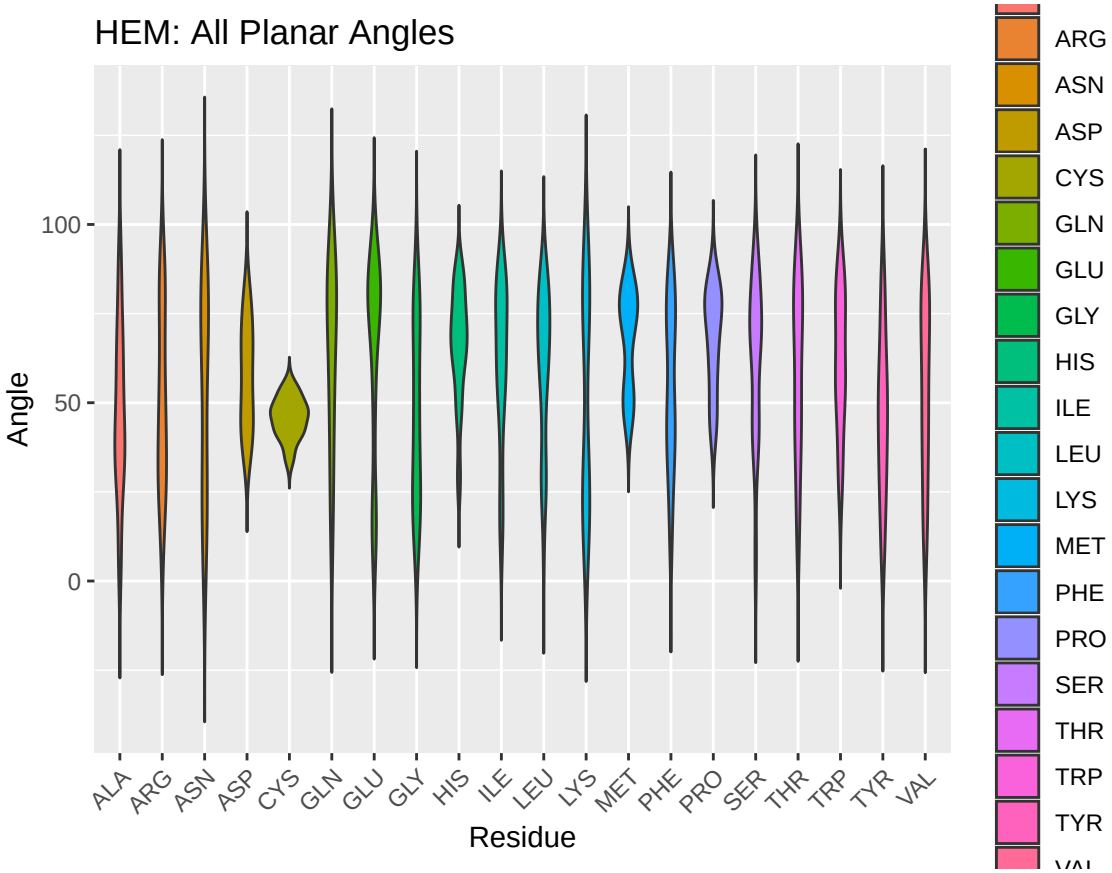

Figure A.25: HEM: All Planar Angles

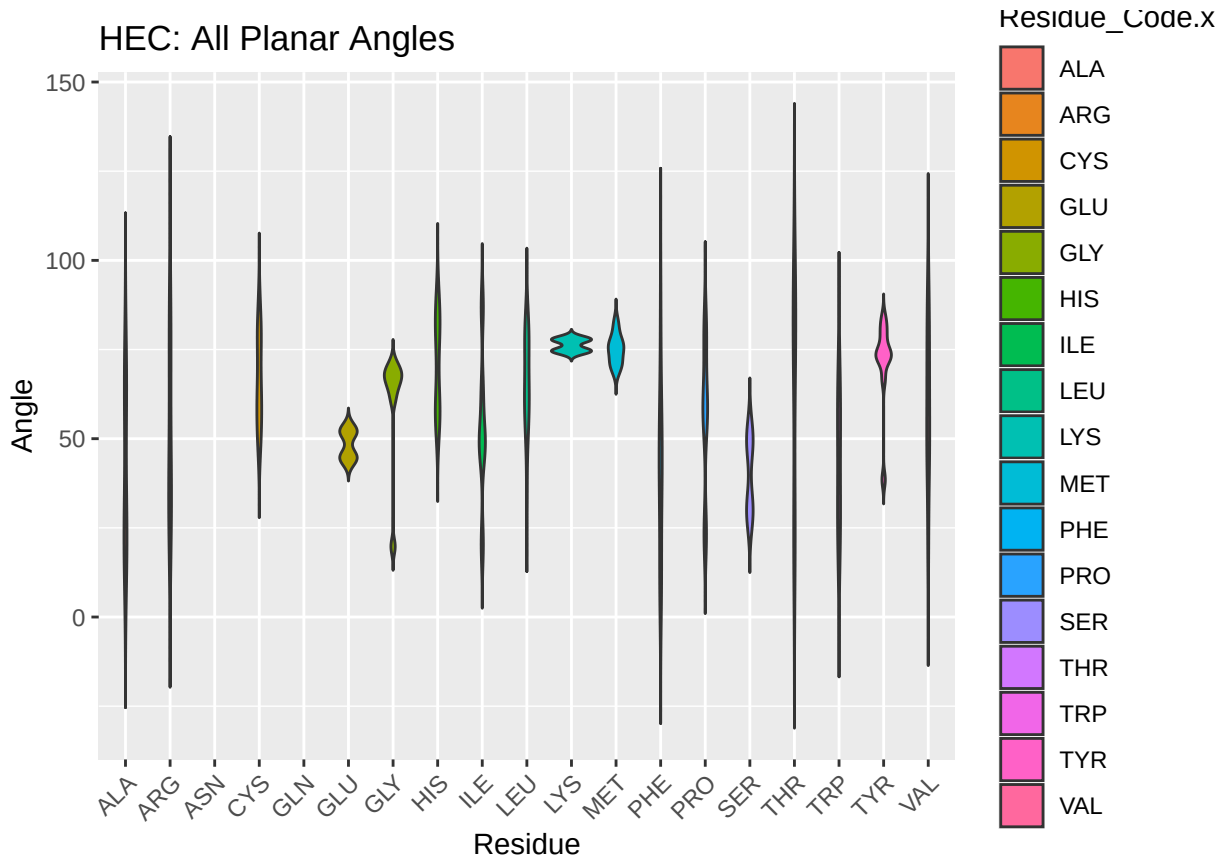

Figure A.26: HEC: All Planar Angles

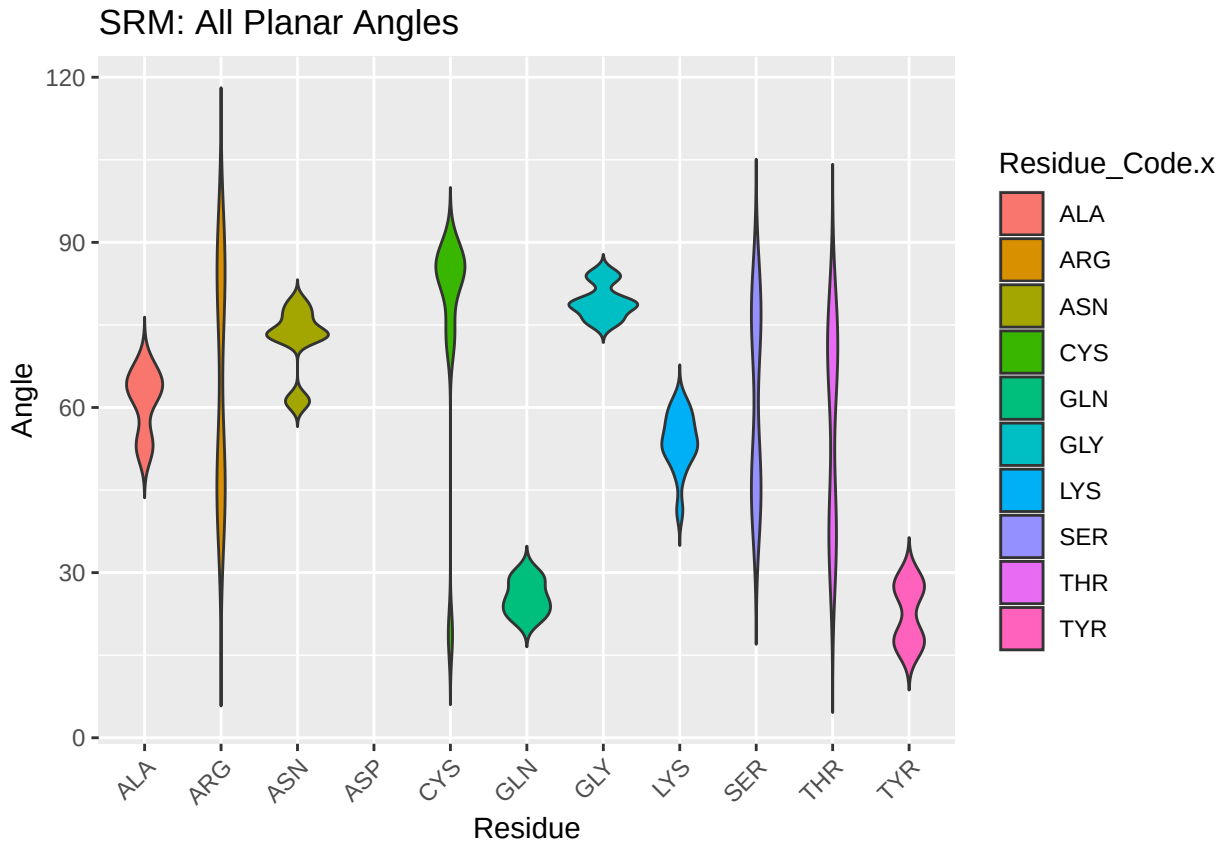

Figure A.27: SRM: All Planar Angles

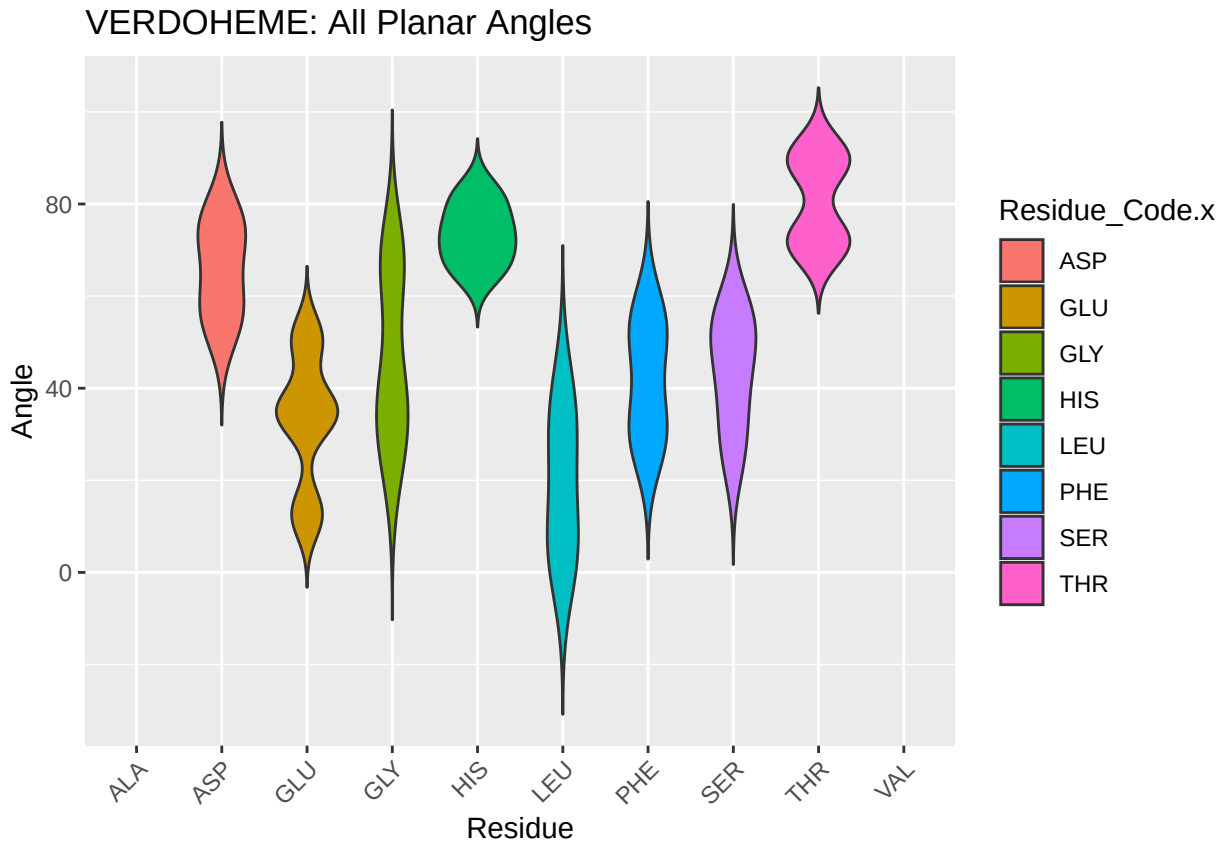

Figure A.28: VERDOHEME: All Planar Angles

Figure A.29: HEM: Planar Angles of Closest Residues

Figure A.30: HEC: Planar Angles of Closest Residues

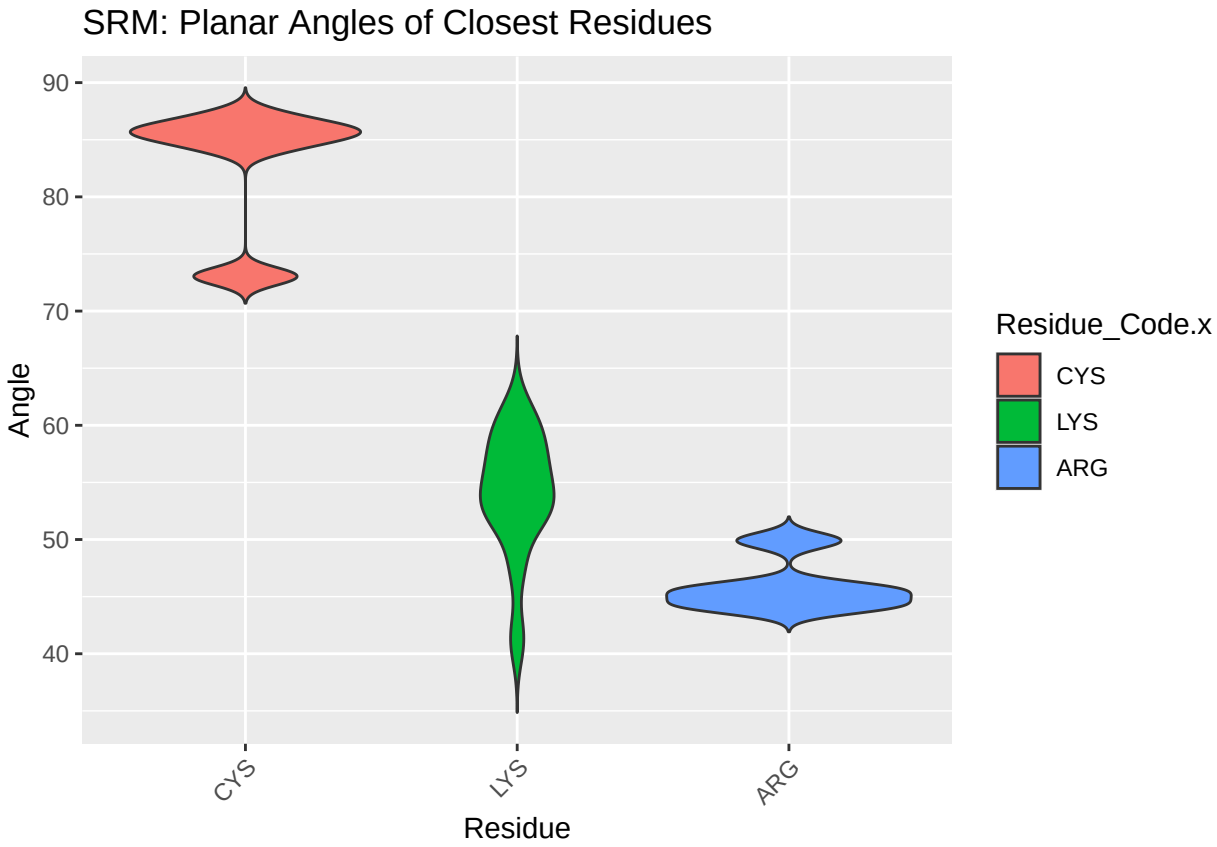

Figure A.31: SRM: Planar Angles of Closest Residues

Figure A.32: VERDOHEME: Planar Angles of Closest Residues

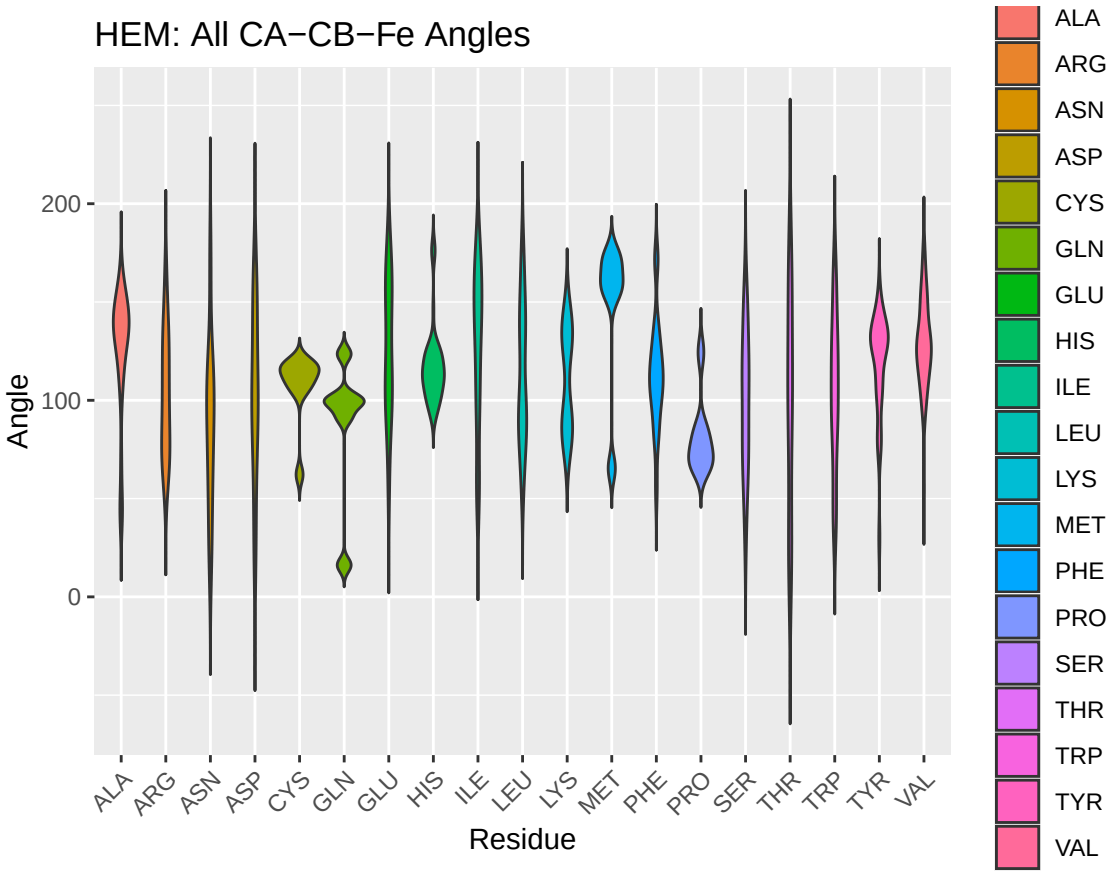

Figure A.33: HEM: All CA-CB-Fe Angles

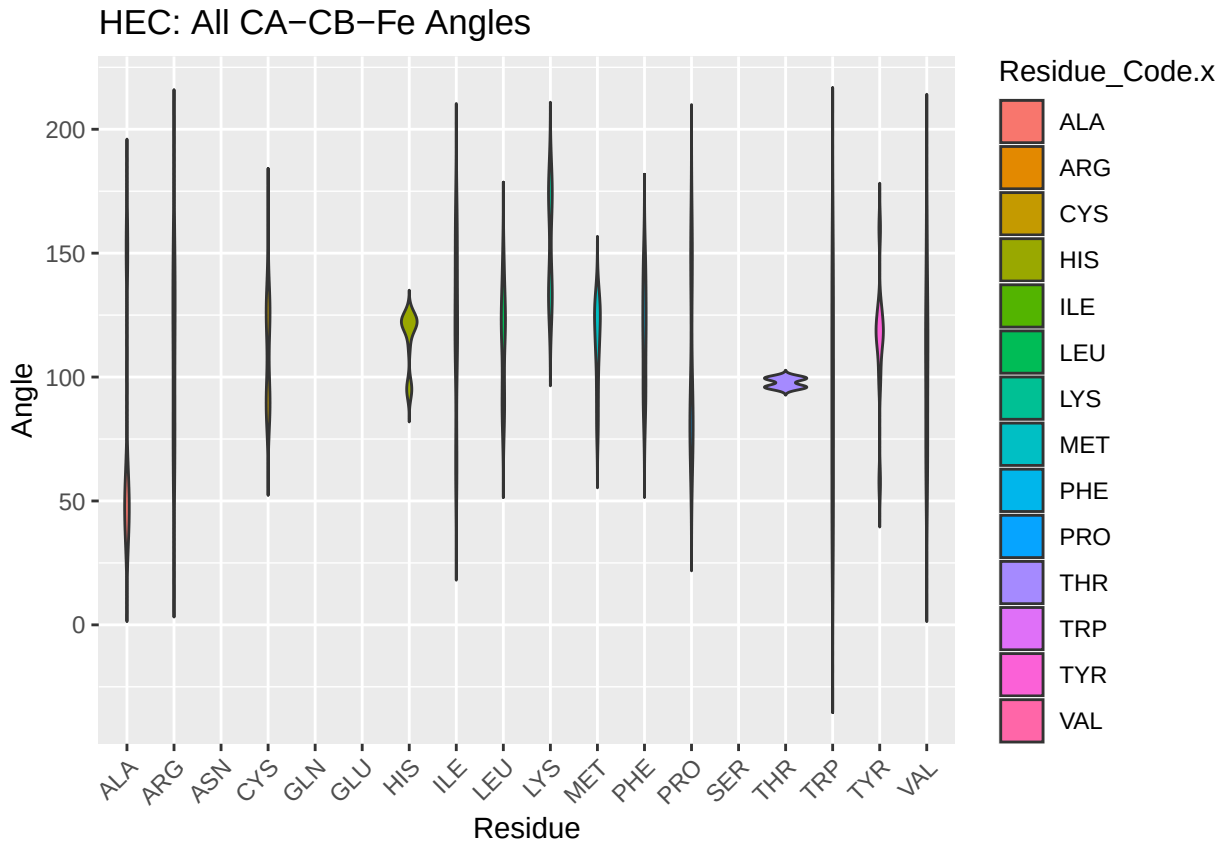

Figure A.34: HEC: All CA-CB-Fe Angles

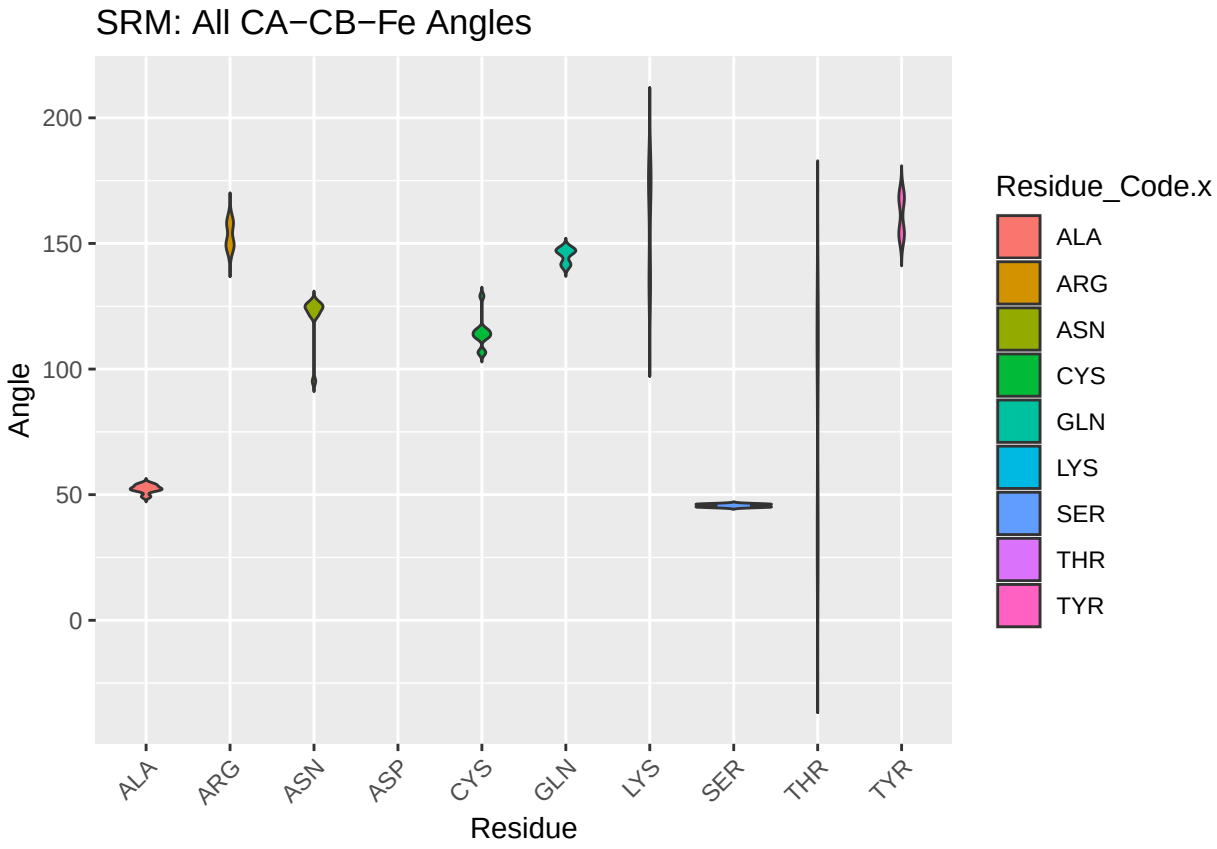

Figure A.35: SRM: All CA-CB-Fe Angles

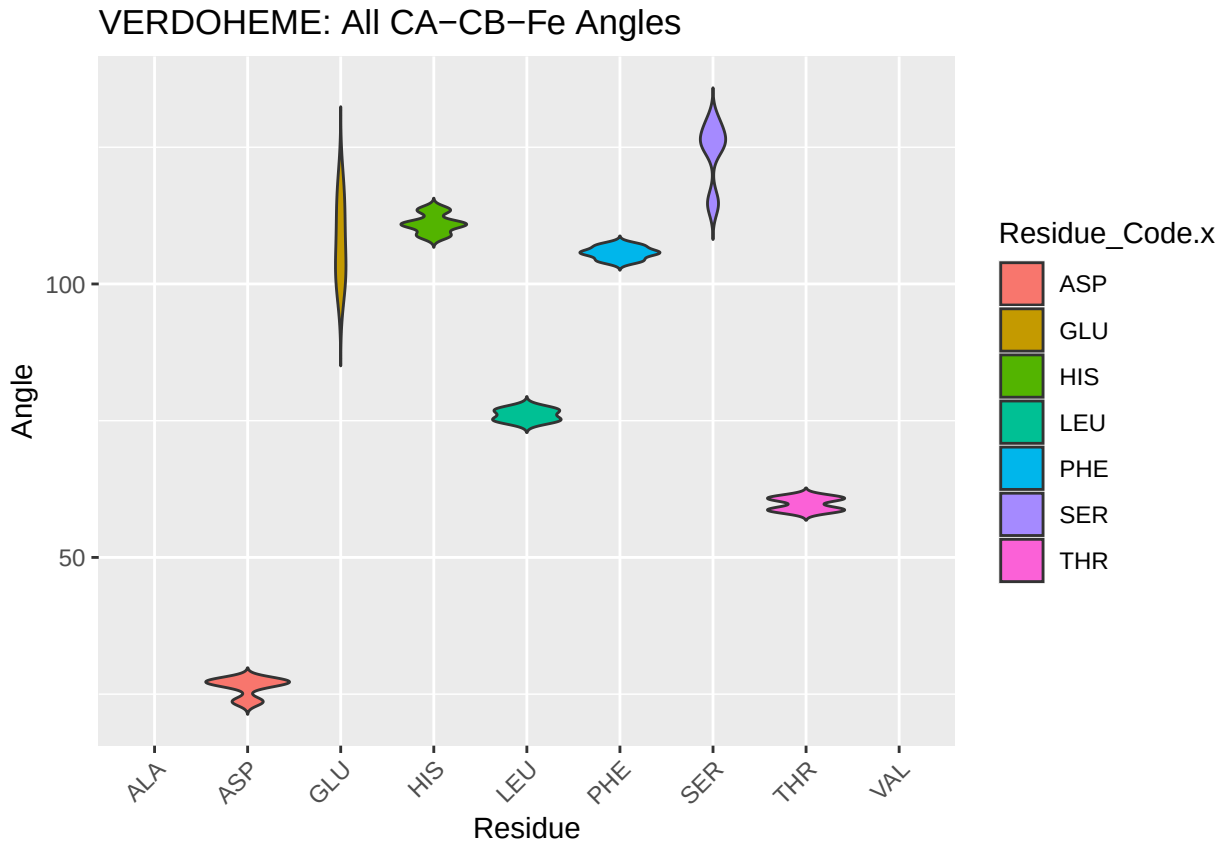

Figure A.36: VERDOHEME: All CA-CB-Fe Angles

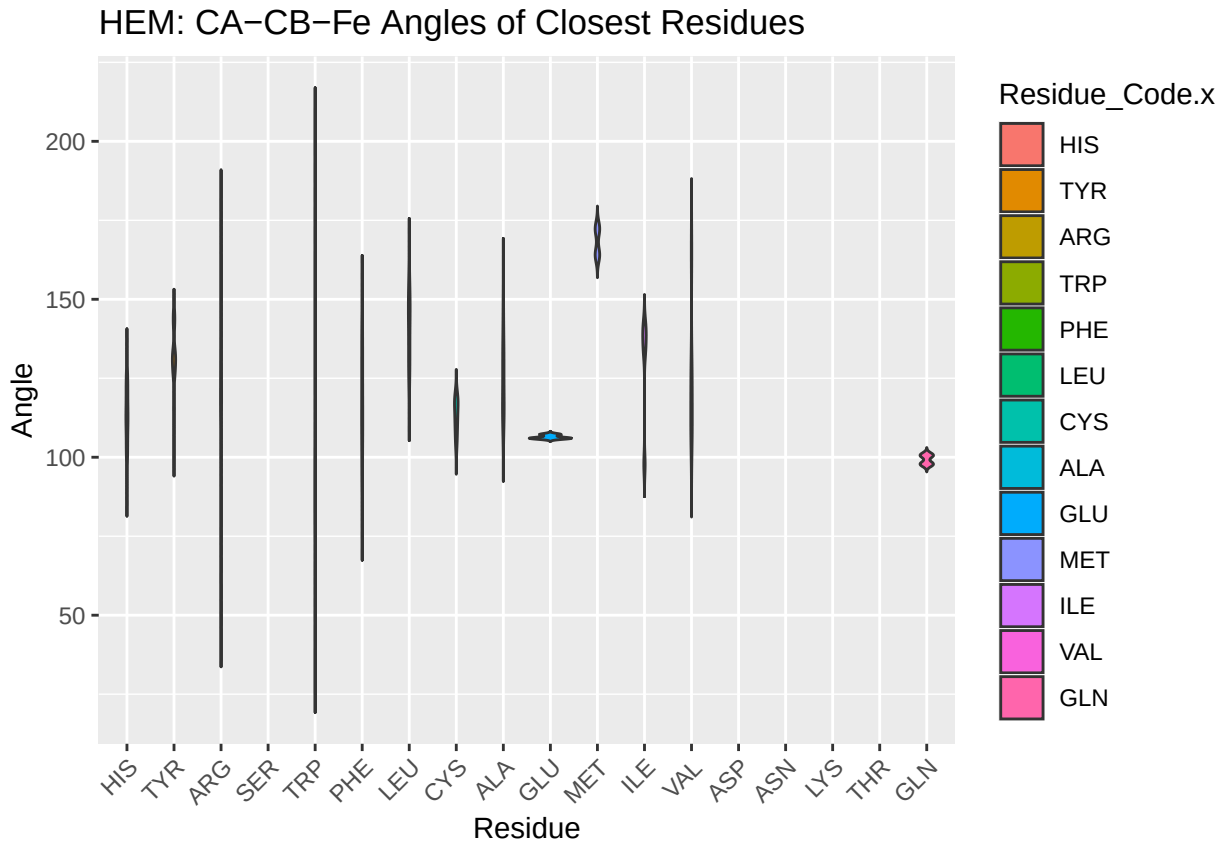

Figure A.37: HEM: CACBFe Angles of Closest Residues

Figure A.38: HEC: CACBFe Angles of Closest Residues

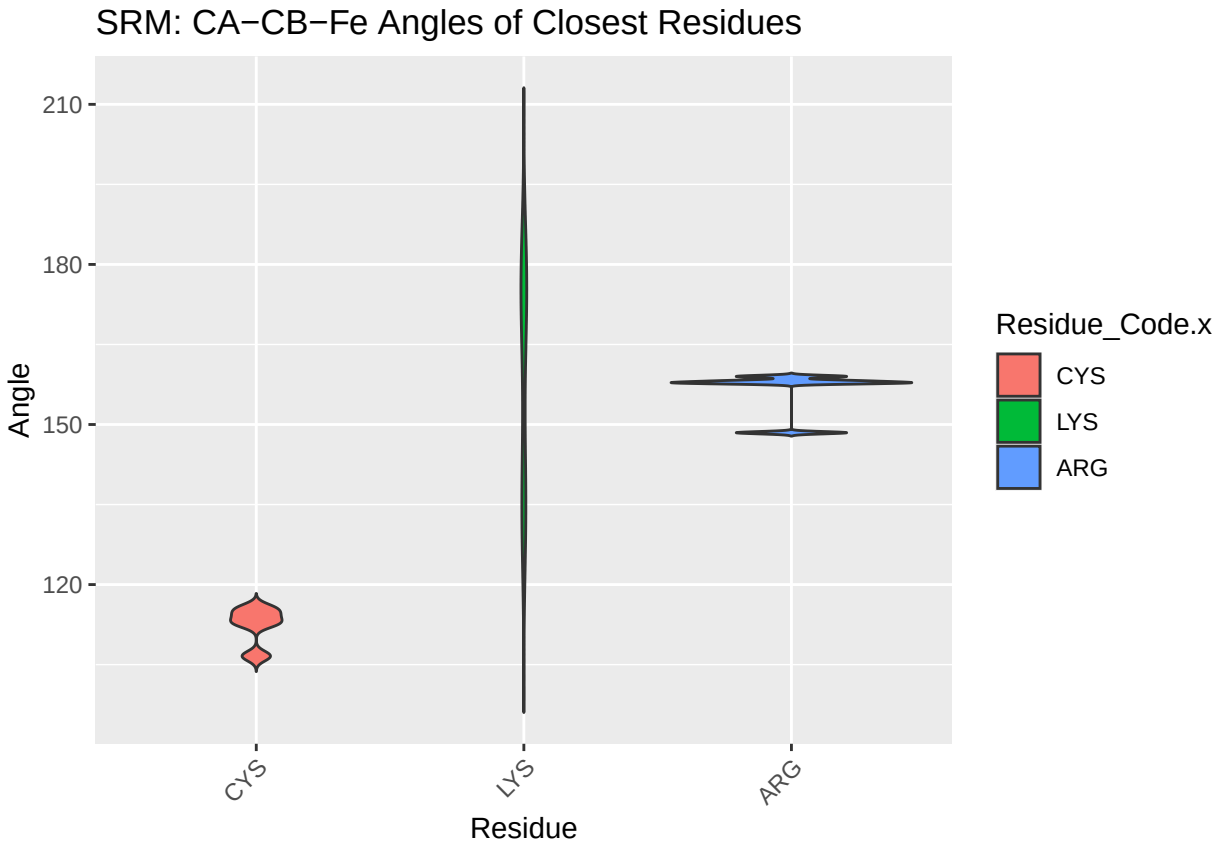

Figure A.39: SRM: CACBFe Angles of Closest Residues

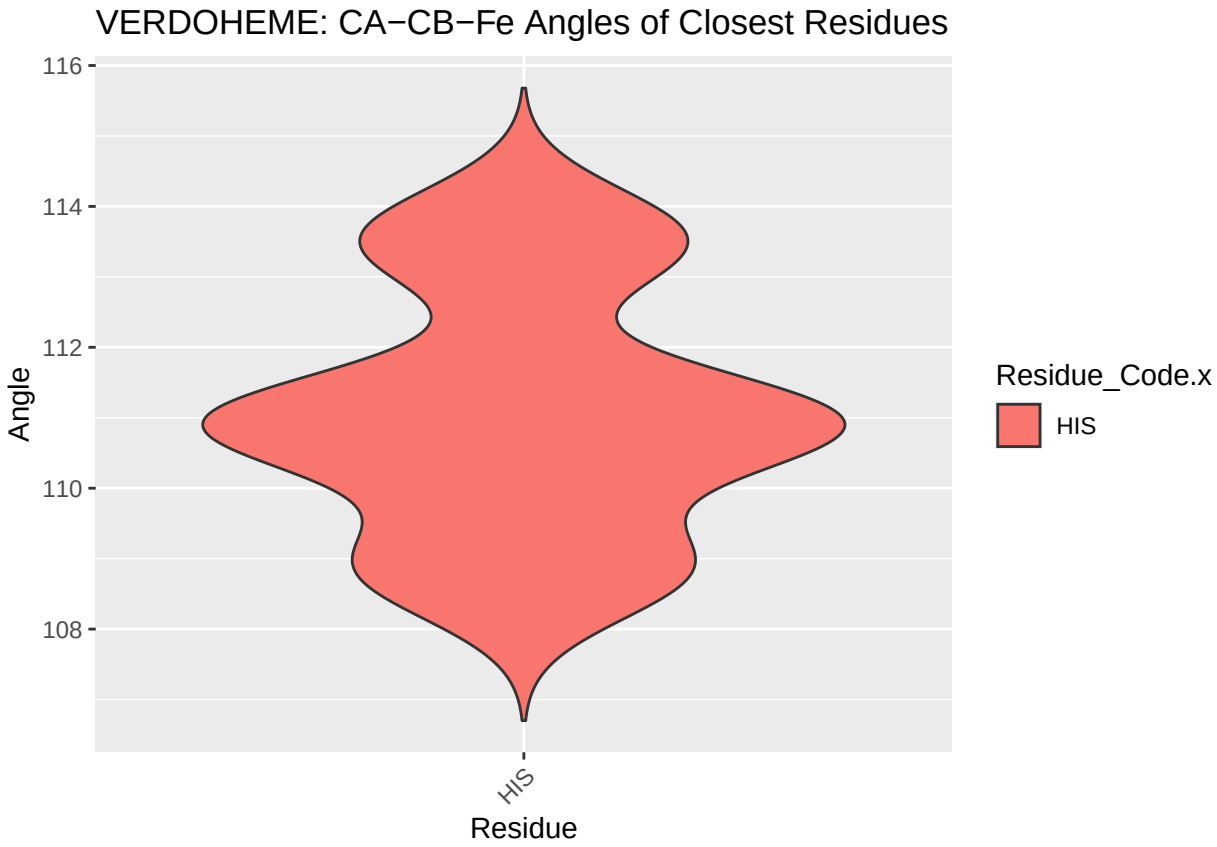

Figure A.40: VERDOHEME: CACBFe Angles of Closest Residues

B
Tables

B.1 Molecule Names and Source Organisms

Table B.1: HEM: Molecules and Source Organisms

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 HPII;	ESCHERICHIA COLI;
1N45	HEME OXYGENASE 1;	HOMO SAPIENS;
1P3T	HEME OXYGENASE 1;	NEISSERIA MENINGITIDIS;

Table B.1: HEM: Molecules and Source Organisms *(continued)*

PDB_ID	Molecule_Name	Source_Organism
1QHU	PROTEIN (HEMOPEXIN);	ORYCTOLAGUS CUNICULUS;
1QJS	HEMOPEXIN;	ORYCTOLAGUS CUNICULUS;
1SI8	CATALASE;	ENTEROCOCCUS FAECALIS;
1SY2	NITROPHORIN 4;	RHODNIUS PROLIXUS;
1U9U	CYTOCHROME B5;	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: HEM: Molecules and Source Organisms *(continued)*

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

Table B.1: HEM: Molecules and Source Organisms *(continued)*

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

Table B.2: HEC: Molecules and Source Organisms

PDB_ID	Molecule_Name	Source_Organism
1BBH	CYTOCHROME C';	ALLOCHROMATIUM VINOSUM;
1S56	HEMOGLOBIN-LIKE PROTEIN HBN;	MYCOBACTERIUM TUBERCULOSIS;
1W2L	CYTOCHROME OXIDASE SUBUNIT II;	RHODOTHERMUS MARINUS;
2BC5	SOLUBLE CYTOCHROME B562;	ESCHERICHIA COLI;
2BH5	CYTOCHROME C-550;	PARACOCCUS VERSUTUS;
3EAH	NITRIC OXIDE SYNTHASE, ENDOTHELIAL;	HOMO SAPIENS;
3X15	CYTOCHROME C552;	AQUIFEX AEOLICUS VF5;
4B2N	70 KDA PROTEIN;	XANTHOMONAS SP.;
5KPF	CYTOCHROME C ISO-1;	SACCHAROMYCES CEREVISIAE;
5LFT	CYTOCHROME C ISO-1;	SACCHAROMYCES CEREVISIAE;
5T8W	CYC1P;	SACCHAROMYCES CEREVISIAE;
6VDQ	3-METHYL-L-TYROSINE PEROXYGENASE;	STREPTOMYCES LAVENDULAE;
6WZA	SOLUBLE CYTOCHROME B562;	ESCHERICHIA COLI;
6XNK	CYTOCHROME C;	HOMO SAPIENS;

Table B.3: SRM: Molecules and Source Organisms

PDB_ID	Molecule_Name	Source_Organism
1ZJ8	PROBABLE FERREDOXIN-DEPENDENT NITRITE REDUCTASE NIRA;	MYCOBACTERIUM TUBERCULOSIS;
2AKJ	FERREDOXIN–NITRITE REDUCTASE, CHLOROPLAST;	SPINACIA OLERACEA;
2AOP	SULFITE REDUCTASE HEMOPROTEIN;	ESCHERICHIA COLI;
3B0G	NITRITE REDUCTASE;	NICOTIANA TABACUM;
3VKP	NITRITE REDUCTASE;	NICOTIANA TABACUM;
3VLX	NITRITE REDUCTASE;	NICOTIANA TABACUM;
3VLY	NITRITE REDUCTASE;	NICOTIANA TABACUM;
3VLZ	NITRITE REDUCTASE;	NICOTIANA TABACUM;
5H8V	SULFITE REDUCTASE [FERREDOXIN], CHLOROPLASTIC;	ZEA MAYS;

Table B.4: VERDOHEME: Molecules and Source Organisms

PDB_ID	Molecule_Name	Source_Organism
2ZVU	HEME OXYGENASE 1;	RATTUS NORVEGICUS;
3MOO	HEME OXYGENASE;	CORYNEBACTERIUM DIPHTHERIAE;
1TWN	HEME OXYGENASE 1;	HOMO SAPIENS;
1TWR	HEME OXYGENASE 1;	HOMO SAPIENS;

B.2 Volume and Surface Areas

Table B.5: HEM: Volume and Surface Areas

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

Table B.5: HEM: Volume and Surface Areas *(continued)*

PDB_ID	Volume_Data	HEM_Excluded_SA	HEM_Accessible_SA	Pocket_Excluded_SA	Pocket_Accessible_SA
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
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

Table B.6: HEC: Volume and Surface Areas

PDB_ID	Volume_Data	HEC_Excluded_SA	HEC_Accessible_SA	Pocket_Excluded_SA	Pocket_Accessible_SA
1BBH	969.51	514.130	829.817	6441.44	7514.06
1S56	1103.60	643.733	1075.840	6711.26	7477.96
1W2L	756.08	702.711	1240.680	5042.58	5485.50
2BC5	1166.20	569.905	997.324	5489.91	6306.02
2BH5	814.15	508.637	844.494	6359.51	6975.70
3EAH	1280.90	993.430	1697.130	18413.40	19313.80
3X15	823.59	496.328	802.584	5722.90	7493.62
4B2N	934.13	1255.940	2122.260	21914.30	22455.80
5KPF	778.79	568.036	1007.680	5485.51	6155.84
5LFT	809.40	1720.870	2719.000	5539.47	6315.96
5T8W	858.74	511.519	848.952	5755.48	6458.40
6VDQ	977.52	510.534	846.299	13399.60	14076.40
6WZA	1040.10	713.997	1095.240	5529.40	6385.75
6XNK	2214.40	499.687	835.610	6737.92	8143.17

Table B.7: SRM: Volume and Surface Areas

PDB_ID	Volume_Data	SRM_Excluded_SA	SRM_Accessible_SA	Pocket_Excluded_SA	Pocket_Accessible_SA
1ZJ8	1960.2	656.508	1036.43	20388.7	21432.8
2AKJ	1810.2	659.667	1041.00	21673.6	20933.7
2AOP	1040.5	682.170	1045.18	18119.8	18016.0
3B0G	1189.9	666.995	1054.40	21496.8	21033.9
3VKP	1178.0	675.050	1049.85	21279.3	20964.9
3VLX	1164.8	667.013	1052.76	21470.0	21037.0
3VLY	1061.8	675.293	1046.41	21476.6	21022.1
3VLZ	1123.2	676.360	1051.40	21433.5	20901.8
5H8V	1360.8	685.850	1052.56	22885.9	22713.3

Table B.8: VERDOHEME: Volume and Surface Areas

PDB_ID	Volume_Data	VERDOHEME_EXCLUDED_SA	VERDOHEME_ACCESSIBLE_SA	POCKET_EXCLUDED_SA	POCKET_ACCESSIBLE_SA
2ZVU	984.51	560.791	969.143	9633.81	10317.3
3MOO	864.48	870.228	1772.07	9371.88	10170.3
1TWN	1145	448.81	759.632	9966.97	10896.8
1TWR	1426	469.982	783.313	9854.01	10775.6

B.3 All Planar Angles

Table B.9: HEM: All Planar Angles

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
1N45	28	ALA	6.981230	51.517	ALA
2CJ0	31	ALA	5.440871	54.576	ALA
2CPO	31	ALA	5.505123	50.842	ALA
2J18	31	ALA	5.457126	52.882	ALA
1SY2	42	ALA	6.006055	38.441	ALA
3MVF	42	ALA	5.827660	37.714	ALA
3TGC	42	ALA	6.033598	36.906	ALA
2O6P	49	ALA	6.356063	33.301	ALA
4B8N	54	ALA	6.390793	40.757	ALA
1B5M	67	ALA	5.797296	4.944	ALA
1ICC	67	ALA	6.085233	8.515	ALA
1U9U	67	ALA	6.016697	3.989	ALA
2CJ0	71	ALA	6.531120	88.775	ALA
2CPO	71	ALA	6.539227	89.067	ALA
2J18	71	ALA	6.477348	89.793	ALA
3HX9	71	ALA	6.230664	24.118	ALA

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
4NL5	71	ALA	6.805378	12.006	ALA
4Y1Q	75	ALA	6.722226	65.239	ALA
1P3T	121	ALA	6.382367	68.509	ALA
3SIK	138	ALA	6.231014	84.490	ALA
3QZN	166	ALA	6.907969	73.637	ALA
2R7A	169	ALA	5.223004	39.141	ALA
6A2J	180	ALA	6.687029	46.961	ALA
2BHJ	191	ALA	6.261711	68.057	ALA
6A2J	220	ALA	5.986896	31.915	ALA
6A2J	259	ALA	6.937825	66.152	ALA
4MYP	282	ALA	6.581195	36.442	ALA
4MYP	293	ALA	6.207799	64.118	ALA
2Q6N	298	ALA	5.672036	28.414	ALA
4I3Q	305	ALA	5.305272	55.811	ALA
5VEU	305	ALA	6.219660	37.021	ALA
1ZVI	412	ALA	6.481380	68.137	ALA
2Q6N	442	ALA	6.935846	35.011	ALA
5VEU	447	ALA	6.667315	35.226	ALA
4I3Q	448	ALA	6.441232	28.736	ALA
4JET	40	ARG	5.660400	8.293	ARG
4XZD	40	ARG	5.892195	23.940	ARG
4Y1Q	40	ARG	5.725205	11.586	ARG
3SIK	54	ARG	6.090293	58.962	ARG
2FC2	61	ARG	6.072553	27.736	ARG
2FC2	65	ARG	6.459491	31.691	ARG
4CDP	100	ARG	5.360373	82.404	ARG
2J0P	102	ARG	5.002395	83.046	ARG
4UZV	105	ARG	6.689489	51.468	ARG
4MF9	112	ARG	5.056393	85.919	ARG
5GJ3	142	ARG	9.016294	44.325	ARG
4JET	144	ARG	6.239587	45.482	ARG
4XZD	144	ARG	6.335714	52.771	ARG
4Y1Q	144	ARG	6.425880	45.332	ARG
2BHJ	193	ARG	5.745098	22.913	ARG
2BHJ	197	ARG	6.221230	38.014	ARG

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
4I3Q	212	ARG	6.392849	65.236	ARG
1QHU	214	ARG	6.588734	53.531	ARG
1QJS	214	ARG	6.249190	87.831	ARG
6A2J	217	ARG	6.781589	69.272	ARG
5GJ3	241	ARG	5.542517	89.231	ARG
2IIZ	242	ARG	5.236889	71.798	ARG
1SI8	333	ARG	5.247624	87.335	ARG
2IPS	348	ARG	6.336679	28.401	ARG
7C74	348	ARG	6.274279	28.825	ARG
7DMR	348	ARG	6.250958	34.360	ARG
1IPH	411	ARG	5.321024	79.235	ARG
1ZVI	414	ARG	5.799426	24.112	ARG
1ZVI	418	ARG	6.259544	32.179	ARG
3HX9	7	ASN	9.030558	67.240	ASN
4NL5	7	ASN	5.402231	60.999	ASN
1B2V	41	ASN	6.894251	9.238	ASN
1DK0	41	ASN	6.870425	7.885	ASN
1P3T	118	ASN	6.625279	81.885	ASN
1SI8	127	ASN	6.666708	88.346	ASN
1IPH	201	ASN	6.396844	80.526	ASN
2BHJ	364	ASN	6.955669	54.701	ASN
2IPS	437	ASN	6.276979	27.543	ASN
7C74	437	ASN	6.653391	27.901	ASN
7DMR	437	ASN	6.591349	28.625	ASN
5VEU	440	ASN	6.408862	78.050	ASN
4I3Q	441	ASN	6.139159	80.458	ASN
1P3T	27	ASP	6.267807	39.072	ASP
2E2Y	64	ASP	6.865050	39.668	ASP
2IPS	108	ASP	5.870986	78.247	ASP
7C74	108	ASP	6.017401	74.114	ASP
7DMR	108	ASP	6.266021	79.901	ASP
5KZL	129	ASP	6.318347	48.961	ASP
1N45	140	ASP	6.389011	51.996	ASP
1VGI	140	ASP	6.566393	62.088	ASP
2IIZ	151	ASP	5.861207	42.941	ASP

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
4CDP	191	ASP	6.789427	37.522	ASP
2J0P	194	ASP	6.862392	50.396	ASP
1QHU	203	ASP	6.920576	64.837	ASP
1QJS	203	ASP	6.878437	64.521	ASP
2IIZ	284	ASP	6.598336	68.375	ASP
2CJ0	29	CYS	4.390905	47.217	CYS
2CPO	29	CYS	4.443549	49.291	CYS
2J18	29	CYS	4.359887	47.527	CYS
2FC2	62	CYS	4.482879	54.005	CYS
1P3T	113	CYS	6.881310	41.741	CYS
2BHJ	194	CYS	4.487497	52.816	CYS
1ZVI	415	CYS	4.181834	46.871	CYS
2Q6N	436	CYS	4.305637	40.993	CYS
5VEU	441	CYS	4.349464	42.614	CYS
4I3Q	442	CYS	4.085782	34.781	CYS
2IPS	105	GLN	5.981590	87.342	GLN
7C74	105	GLN	5.667218	84.879	GLN
7DMR	105	GLN	5.517249	82.031	GLN
5GJ3	141	GLN	9.940999	57.821	GLN
2R7A	253	GLN	6.081153	19.452	GLN
6A2J	258	GLN	5.803666	43.028	GLN
4MYP	292	GLN	6.537566	73.527	GLN
5KZL	19	GLU	5.803913	14.669	GLU
1N45	29	GLU	6.277510	13.488	GLU
1VGI	29	GLU	6.279863	19.844	GLU
5O1L	148	GLU	6.440638	81.093	GLU
2CJ0	183	GLU	5.716050	77.664	GLU
2CPO	183	GLU	5.799506	78.548	GLU
2J18	183	GLU	5.722472	78.531	GLU
1QHU	225	GLU	6.177350	81.356	GLU
1QJS	226	GLU	6.465511	78.730	GLU
2IPS	258	GLU	6.388898	83.283	GLU
7C74	258	GLU	6.258582	88.863	GLU
7DMR	258	GLU	6.172262	88.960	GLU
2Q6N	439	GLU	6.270464	60.625	GLU

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
1ZVI	592	GLU	6.601349	48.481	GLU
1B5M	41	GLY	5.388127	72.708	GLY
1ICC	41	GLY	5.723853	72.752	GLY
1U9U	41	GLY	5.723510	83.944	GLY
1B5M	42	GLY	6.533917	10.848	GLY
1ICC	42	GLY	6.657462	8.777	GLY
1U9U	42	GLY	6.689632	17.633	GLY
4B8N	50	GLY	5.464969	87.471	GLY
4B8N	51	GLY	6.462950	23.037	GLY
1B5M	62	GLY	6.365897	81.093	GLY
2FC2	64	GLY	5.882725	21.989	GLY
1P3T	116	GLY	5.737222	80.192	GLY
1P3T	120	GLY	4.843774	41.129	GLY
5KZL	128	GLY	5.130966	70.591	GLY
5KZL	132	GLY	5.705062	50.430	GLY
1N45	139	GLY	5.251379	58.119	GLY
1VGI	139	GLY	5.155470	60.437	GLY
1N45	143	GLY	5.882948	37.778	GLY
1VGI	143	GLY	5.279720	32.760	GLY
1VGI	144	GLY	5.974807	66.493	GLY
2R7A	170	GLY	5.922307	19.803	GLY
6A2J	179	GLY	5.548597	36.551	GLY
2BHJ	196	GLY	5.667103	19.625	GLY
2FC2	233	GLY	6.517575	77.972	GLY
6A2J	262	GLY	5.820895	75.177	GLY
4MYP	291	GLY	6.624699	50.662	GLY
2Q6N	299	GLY	6.518431	10.616	GLY
4I3Q	306	GLY	6.573103	20.924	GLY
2IPS	350	GLY	6.712596	52.440	GLY
7C74	350	GLY	6.606591	46.520	GLY
7DMR	350	GLY	6.694618	48.519	GLY
2BHJ	365	GLY	6.617587	80.698	GLY
1ZVI	417	GLY	5.404983	24.763	GLY
2Q6N	438	GLY	5.615678	28.366	GLY
5VEU	443	GLY	5.482822	27.362	GLY

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
4I3Q	444	GLY	5.222394	22.218	GLY
1ZVI	586	GLY	6.997972	72.788	GLY
5KZL	15	HIS	4.819650	59.949	HIS
1P3T	23	HIS	4.573926	67.542	HIS
1N45	25	HIS	4.545004	69.116	HIS
1VGI	25	HIS	4.646180	72.142	HIS
1B2V	32	HIS	4.667618	51.415	HIS
1DK0	32	HIS	4.556145	48.497	HIS
1DKH	32	HIS	5.099382	50.187	HIS
1B5M	39	HIS	4.456809	87.693	HIS
1ICC	39	HIS	4.542187	78.752	HIS
1U9U	39	HIS	4.589294	80.451	HIS
4B8N	48	HIS	4.479396	87.524	HIS
1SI8	54	HIS	5.688888	26.890	HIS
1SY2	59	HIS	4.045387	85.351	HIS
3MVF	59	HIS	4.066882	87.977	HIS
3TGC	59	HIS	4.100823	87.207	HIS
1B5M	63	HIS	4.211990	71.272	HIS
1ICC	63	HIS	4.451283	57.814	HIS
1U9U	63	HIS	4.417873	66.393	HIS
2SPL	64	HIS	5.889080	73.719	HIS
5CN5	64	HIS	5.804727	84.840	HIS
4B8N	71	HIS	4.416116	70.933	HIS
3VP5	72	HIS	4.371971	45.918	HIS
3HX9	75	HIS	4.195649	50.709	HIS
4NL5	75	HIS	4.473936	46.347	HIS
4JET	81	HIS	5.381133	54.183	HIS
4XZD	81	HIS	5.263108	67.684	HIS
4Y1Q	81	HIS	5.294289	61.474	HIS
1B2V	83	HIS	5.366599	56.778	HIS
1DK0	83	HIS	5.314133	62.320	HIS
1DKH	83	HIS	5.223800	43.522	HIS
2CN4	83	HIS	5.251875	61.039	HIS
3QZN	83	HIS	4.660500	67.495	HIS
2E2Y	93	HIS	4.514535	86.534	HIS

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
2SPL	93	HIS	4.578545	88.954	HIS
5CN5	93	HIS	4.575365	82.799	HIS
2E2Y	97	HIS	5.917056	68.715	HIS
2SPL	97	HIS	5.997752	67.846	HIS
5CN5	97	HIS	5.966408	71.762	HIS
4UZV	106	HIS	4.502311	79.507	HIS
2IPS	109	HIS	5.924623	73.103	HIS
7C74	109	HIS	5.952700	70.733	HIS
7DMR	109	HIS	5.699226	62.306	HIS
2VEB	120	HIS	4.471709	79.839	HIS
3QZZ	120	HIS	4.599066	74.693	HIS
3ZJS	120	HIS	4.427156	73.923	HIS
1IPH	128	HIS	5.713777	33.997	HIS
2O6P	134	HIS	6.496593	61.077	HIS
3VP5	149	HIS	4.350835	49.264	HIS
3QZN	168	HIS	6.973181	70.767	HIS
4CDP	193	HIS	4.417630	74.031	HIS
2J0P	196	HIS	4.310325	75.104	HIS
5O1L	198	HIS	4.305405	66.467	HIS
5O1M	198	HIS	4.392715	64.463	HIS
4MF9	209	HIS	4.606487	63.203	HIS
1QHU	213	HIS	4.734866	79.430	HIS
1QJS	213	HIS	4.696712	82.802	HIS
6A2J	216	HIS	4.601722	63.468	HIS
1QHU	222	HIS	6.740296	77.401	HIS
2IIZ	224	HIS	4.533607	61.464	HIS
1QHU	265	HIS	4.200094	83.910	HIS
1QJS	266	HIS	4.484379	82.026	HIS
6A2J	278	HIS	4.655598	63.931	HIS
2IPS	351	HIS	4.125792	28.391	HIS
7C74	351	HIS	4.494179	25.953	HIS
7DMR	351	HIS	4.201640	31.126	HIS
3HX9	9	ILE	9.558396	78.071	ILE
4NL5	9	ILE	5.756873	80.656	ILE
4JET	30	ILE	6.988601	55.096	ILE

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
2O6P	48	ILE	5.365972	44.466	ILE
4B8N	55	ILE	5.758462	70.943	ILE
2FC2	63	ILE	6.106378	69.135	ILE
2E2Y	68	ILE	5.517060	80.623	ILE
3VP5	71	ILE	6.407016	71.208	ILE
2E2Y	99	ILE	6.130795	52.979	ILE
2SPL	99	ILE	6.223033	48.696	ILE
5CN5	99	ILE	6.410362	54.086	ILE
2E2Y	107	ILE	6.704700	16.195	ILE
2SPL	107	ILE	6.505472	17.465	ILE
5CN5	107	ILE	6.767432	16.093	ILE
4UZV	111	ILE	5.897899	46.982	ILE
2Q6N	114	ILE	6.560571	9.779	ILE
2VEB	116	ILE	6.573571	81.358	ILE
3QZZ	116	ILE	6.472356	81.312	ILE
3ZJS	116	ILE	6.518950	85.700	ILE
2O6P	121	ILE	6.852081	79.662	ILE
3SIK	129	ILE	6.189129	72.935	ILE
3SIK	131	ILE	6.481115	75.292	ILE
2VEB	137	ILE	6.361213	61.323	ILE
3QZZ	137	ILE	6.393964	65.377	ILE
3ZJS	137	ILE	6.315026	65.712	ILE
3QZN	159	ILE	5.866079	87.212	ILE
3QZN	164	ILE	6.384201	78.779	ILE
2BHJ	195	ILE	6.216303	34.244	ILE
2FC2	214	ILE	6.545905	59.848	ILE
5O1L	222	ILE	6.024951	24.897	ILE
5O1M	222	ILE	6.241067	30.392	ILE
2IIZ	225	ILE	6.430481	80.524	ILE
5O1L	227	ILE	6.973430	56.638	ILE
4CDP	252	ILE	6.178209	87.181	ILE
2J0P	255	ILE	6.197370	88.613	ILE
6A2J	265	ILE	6.271826	86.089	ILE
4MF9	268	ILE	6.092502	87.522	ILE
2Q6N	363	ILE	6.794813	63.519	ILE

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
2Q6N	435	ILE	6.531691	62.893	ILE
5VEU	442	ILE	6.119535	59.766	ILE
4I3Q	443	ILE	5.985023	55.615	ILE
2CJ0	32	LEU	5.757197	86.436	LEU
2CPO	32	LEU	5.913058	85.779	LEU
2J18	32	LEU	5.760472	86.600	LEU
1B5M	46	LEU	5.848737	58.371	LEU
1ICC	46	LEU	5.941384	55.221	LEU
1U9U	46	LEU	5.958763	65.230	LEU
1SY2	57	LEU	6.145372	80.845	LEU
3MVF	57	LEU	6.242544	82.824	LEU
3TGC	57	LEU	6.147624	82.612	LEU
4B8N	70	LEU	6.456250	84.030	LEU
1B2V	77	LEU	6.429830	74.863	LEU
1DK0	77	LEU	6.502332	70.907	LEU
1DKH	77	LEU	6.345588	81.197	LEU
2CN4	77	LEU	6.548785	64.950	LEU
4UZV	79	LEU	6.352126	32.691	LEU
2E2Y	89	LEU	6.167984	57.194	LEU
2SPL	89	LEU	6.446644	54.572	LEU
5CN5	89	LEU	6.607510	81.740	LEU
4CDP	90	LEU	6.499175	53.089	LEU
4UZV	102	LEU	6.801707	80.742	LEU
2E2Y	104	LEU	6.384225	42.486	LEU
2SPL	104	LEU	6.518599	49.950	LEU
5CN5	104	LEU	6.517400	40.971	LEU
1P3T	119	LEU	6.709401	29.938	LEU
1SY2	123	LEU	5.902915	71.098	LEU
3MVF	123	LEU	5.891492	77.839	LEU
3TGC	123	LEU	5.908675	73.018	LEU
5KZL	127	LEU	6.731689	26.021	LEU
1SY2	133	LEU	6.241713	67.620	LEU
3MVF	133	LEU	6.341681	74.740	LEU
3TGC	133	LEU	6.315080	69.684	LEU
5KZL	136	LEU	6.422701	84.272	LEU

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
1N45	138	LEU	6.717099	17.508	LEU
1VGI	138	LEU	6.110494	28.406	LEU
2VEB	142	LEU	6.331426	30.581	LEU
3QZZ	142	LEU	6.534813	26.402	LEU
3ZJS	142	LEU	6.289922	24.952	LEU
1N45	147	LEU	6.115862	65.024	LEU
2R7A	167	LEU	6.508147	65.218	LEU
5O1L	171	LEU	5.743071	78.726	LEU
2IIZ	255	LEU	6.075868	6.622	LEU
2R7A	257	LEU	5.559331	26.488	LEU
2IIZ	286	LEU	5.566800	60.469	LEU
2IPS	417	LEU	6.792313	68.323	LEU
2IPS	433	LEU	5.458537	63.062	LEU
7C74	433	LEU	5.275537	56.669	LEU
7DMR	433	LEU	5.225161	71.791	LEU
2Q6N	437	LEU	5.864970	68.730	LEU
3VP5	145	LYS	5.832567	22.419	LYS
5O1M	167	LYS	5.125712	80.116	LYS
3QZN	84	MET	6.337233	82.368	MET
1B2V	140	MET	6.218846	78.617	MET
1DK0	140	MET	6.185917	75.977	MET
1DKH	140	MET	6.519598	80.084	MET
2CN4	140	MET	5.816277	79.067	MET
4JET	147	MET	5.810508	82.720	MET
4XZD	147	MET	6.297861	74.779	MET
4Y1Q	147	MET	6.115760	72.668	MET
4UZV	151	MET	5.908059	50.673	MET
4CDP	241	MET	6.340896	51.184	MET
2J0P	244	MET	6.821994	47.273	MET
4MF9	257	MET	6.826627	47.678	MET
5VEU	444	MET	6.285199	69.820	MET
4I3Q	445	MET	5.975507	54.809	MET
3HX9	23	PHE	8.679990	57.262	PHE
4NL5	23	PHE	5.580423	79.989	PHE
2SPL	29	PHE	6.129536	67.992	PHE

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
1B5M	35	PHE	5.848448	51.666	PHE
1ICC	35	PHE	6.276818	51.071	PHE
1U9U	35	PHE	6.094672	55.366	PHE
2SPL	43	PHE	5.815167	43.358	PHE
5CN5	43	PHE	5.981197	45.242	PHE
4B8N	44	PHE	6.120000	52.229	PHE
4JET	50	PHE	6.875792	36.195	PHE
4Y1Q	50	PHE	6.555816	41.424	PHE
4UZV	53	PHE	6.941930	87.835	PHE
2CJ0	57	PHE	6.484645	35.572	PHE
2CPO	57	PHE	6.473913	37.630	PHE
2J18	57	PHE	6.534471	36.396	PHE
1B5M	58	PHE	6.096500	79.544	PHE
1ICC	58	PHE	6.182239	87.840	PHE
4B8N	67	PHE	6.248829	74.088	PHE
4UZV	67	PHE	5.984317	67.843	PHE
1SY2	68	PHE	6.098374	86.062	PHE
3MVF	68	PHE	6.146303	85.237	PHE
3TGC	68	PHE	6.152796	84.376	PHE
2VEB	74	PHE	6.405384	85.523	PHE
3QZZ	74	PHE	6.218919	81.733	PHE
3ZJS	74	PHE	6.270262	76.080	PHE
3VP5	76	PHE	6.844578	44.869	PHE
4JET	77	PHE	6.310922	82.490	PHE
4XZD	77	PHE	6.275751	87.170	PHE
4Y1Q	77	PHE	6.412846	87.126	PHE
2VEB	93	PHE	5.810118	22.043	PHE
3QZZ	93	PHE	6.033470	11.038	PHE
3ZJS	93	PHE	5.922481	16.833	PHE
2CJ0	103	PHE	6.182880	27.021	PHE
2CPO	103	PHE	6.396792	28.962	PHE
2J18	103	PHE	6.235843	27.909	PHE
3VP5	112	PHE	6.509162	68.707	PHE
4UZV	119	PHE	5.820671	52.586	PHE
1SI8	132	PHE	6.553242	35.834	PHE

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
1SI8	140	PHE	5.575451	44.222	PHE
2VEB	145	PHE	6.211153	71.125	PHE
3QZZ	145	PHE	6.192963	67.209	PHE
3ZJS	145	PHE	6.059949	63.965	PHE
1P3T	181	PHE	5.974488	28.002	PHE
2CJ0	186	PHE	5.833496	74.907	PHE
2CPO	186	PHE	5.891089	74.604	PHE
2J18	186	PHE	5.882819	73.963	PHE
5KZL	195	PHE	6.351090	26.366	PHE
2J0P	199	PHE	6.468406	77.213	PHE
1IPH	206	PHE	6.665963	47.799	PHE
1N45	207	PHE	5.975984	35.914	PHE
1VGI	207	PHE	6.238995	35.601	PHE
1IPH	214	PHE	5.767678	38.797	PHE
2FC2	231	PHE	6.129726	47.062	PHE
4CDP	243	PHE	5.994465	75.432	PHE
2J0P	246	PHE	6.155004	71.919	PHE
2IIZ	257	PHE	5.749045	43.524	PHE
4MF9	259	PHE	5.680334	67.502	PHE
7C74	347	PHE	6.478230	66.212	PHE
7DMR	347	PHE	6.671472	71.799	PHE
2BHJ	363	PHE	5.980185	49.593	PHE
2Q6N	429	PHE	6.192258	16.599	PHE
5VEU	434	PHE	6.084164	6.989	PHE
4I3Q	435	PHE	6.161681	12.310	PHE
1ZVI	584	PHE	6.009975	47.157	PHE
2CJ0	28	PRO	6.127671	77.384	PRO
2CPO	28	PRO	6.018197	79.394	PRO
2J18	28	PRO	6.103023	75.350	PRO
2CJ0	30	PRO	5.960531	45.202	PRO
2CPO	30	PRO	6.017188	43.004	PRO
2J18	30	PRO	5.936382	46.559	PRO
1B5M	40	PRO	6.032548	64.686	PRO
1ICC	40	PRO	6.016737	74.979	PRO
1U9U	40	PRO	6.149502	62.201	PRO

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
4B8N	49	PRO	6.182011	55.551	PRO
1SI8	315	PRO	6.539721	79.646	PRO
1IPH	393	PRO	6.703993	79.546	PRO
2Q6N	428	PRO	6.945175	64.749	PRO
5VEU	433	PRO	6.574196	84.362	PRO
4I3Q	434	PRO	6.893037	81.173	PRO
1B2V	42	SER	6.443386	37.867	SER
1DK0	42	SER	6.540219	66.931	SER
1DKH	42	SER	6.070312	84.431	SER
2FC2	59	SER	6.581787	68.948	SER
2E2Y	92	SER	6.454585	87.015	SER
2SPL	92	SER	6.650791	83.681	SER
5CN5	92	SER	6.529632	89.481	SER
1P3T	117	SER	5.531584	72.173	SER
5GJ3	124	SER	10.238794	71.645	SER
5KZL	131	SER	6.438631	67.739	SER
1N45	142	SER	6.525024	45.908	SER
1VGI	142	SER	5.700272	44.929	SER
4MYP	205	SER	6.655356	71.936	SER
6A2J	261	SER	6.949581	69.073	SER
1QHU	266	SER	6.680148	46.159	SER
1QJS	267	SER	6.730283	37.983	SER
1IPH	414	SER	6.728176	7.127	SER
1DK0	33	THR	6.991008	82.730	THR
2R7A	52	THR	5.945515	75.272	THR
2E2Y	67	THR	6.891096	23.524	THR
3VP5	68	THR	6.164947	65.743	THR
4XZD	82	THR	6.830323	42.191	THR
1B2V	84	THR	6.798527	48.773	THR
1DK0	84	THR	6.799510	46.371	THR
1DKH	84	THR	6.267175	13.394	THR
2CN4	84	THR	6.804573	47.318	THR
1SY2	121	THR	6.333312	76.088	THR
3MVF	121	THR	6.595150	73.083	THR
3TGC	121	THR	6.343084	72.698	THR

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
3VP5	130	THR	5.980868	66.884	THR
1N45	135	THR	6.713859	87.717	THR
1VGI	135	THR	6.883314	86.934	THR
5O1M	168	THR	6.373467	86.011	THR
6A2J	178	THR	6.772182	40.134	THR
5O1L	194	THR	6.305648	88.159	THR
5O1M	194	THR	6.409916	87.811	THR
4MF9	208	THR	6.202558	72.980	THR
5O1L	230	THR	6.574103	56.973	THR
5O1M	230	THR	6.603918	48.514	THR
2Q6N	302	THR	5.748396	11.940	THR
4I3Q	309	THR	6.214341	29.056	THR
5VEU	309	THR	5.895842	31.467	THR
2E2Y	43	TRP	5.845537	63.663	TRP
2FC2	56	TRP	5.737975	58.198	TRP
3QZZ	60	TRP	6.491833	87.108	TRP
3ZJS	60	TRP	6.366999	80.062	TRP
3HX9	66	TRP	7.852796	51.391	TRP
4NL5	66	TRP	6.235302	53.548	TRP
2R7A	68	TRP	6.192116	56.988	TRP
1QHU	171	TRP	6.147194	45.734	TRP
1QJS	171	TRP	6.211700	40.663	TRP
2VEB	185	TRP	5.717992	82.552	TRP
3QZZ	185	TRP	6.111800	87.248	TRP
3ZJS	185	TRP	5.960798	85.251	TRP
2BHJ	188	TRP	6.049049	55.507	TRP
2CJ0	213	TRP	6.764355	72.064	TRP
2J18	213	TRP	6.782850	71.352	TRP
2FC2	234	TRP	6.837576	33.085	TRP
1QHU	267	TRP	5.987630	76.604	TRP
1QJS	268	TRP	6.230710	77.078	TRP
2BHJ	366	TRP	6.764735	26.115	TRP
1ZVI	409	TRP	5.660275	56.622	TRP
1ZVI	587	TRP	6.843603	29.680	TRP
1SY2	40	TYR	5.887937	30.456	TYR

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
3MVF	40	TYR	6.759408	4.606	TYR
3TGC	40	TYR	5.967215	29.632	TYR
2O6P	52	TYR	6.682161	77.760	TYR
2CN4	55	TYR	6.806239	16.581	TYR
4JET	55	TYR	6.877273	11.357	TYR
4XZD	55	TYR	6.821652	12.231	TYR
4Y1Q	55	TYR	6.699820	8.751	TYR
1SY2	58	TYR	6.964531	86.657	TYR
1U9U	58	TYR	6.232812	76.301	TYR
3ZJS	61	TYR	6.548411	42.808	TYR
2R7A	67	TYR	4.159993	73.259	TYR
1B2V	75	TYR	4.251885	39.160	TYR
1DK0	75	TYR	4.346840	40.042	TYR
1DKH	75	TYR	4.792830	45.976	TYR
2CN4	75	TYR	4.345054	45.523	TYR
4JET	75	TYR	4.420106	47.089	TYR
4XZD	75	TYR	4.329954	46.839	TYR
3QZN	87	TYR	6.251729	84.821	TYR
3VP5	91	TYR	6.574739	32.406	TYR
2O6P	132	TYR	4.055037	56.191	TYR
2O6P	136	TYR	5.148558	86.464	TYR
3SIK	136	TYR	4.260470	52.942	TYR
1B2V	137	TYR	6.232518	27.438	TYR
1DK0	137	TYR	6.186950	32.086	TYR
1DKH	137	TYR	6.409147	26.390	TYR
2CN4	137	TYR	6.142879	28.073	TYR
3SIK	140	TYR	5.120136	63.829	TYR
5GJ3	140	TYR	7.520130	58.494	TYR
3QZN	170	TYR	5.718488	72.518	TYR
1QHU	204	TYR	6.239544	47.589	TYR
1QJS	204	TYR	6.225721	48.525	TYR
5GJ3	239	TYR	4.170326	62.993	TYR
4MYP	280	TYR	4.465249	56.836	TYR
4MYP	289	TYR	5.900895	20.187	TYR
1SI8	337	TYR	3.976560	58.339	TYR

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
1IPH	415	TYR	4.218561	62.200	TYR
1P3T	26	VAL	6.716946	70.533	VAL
1SY2	36	VAL	6.479806	81.825	VAL
3TGC	36	VAL	6.135653	80.270	VAL
1B2V	37	VAL	5.425221	76.657	VAL
1DK0	37	VAL	5.400636	79.308	VAL
1DKH	37	VAL	5.642973	85.568	VAL
1B5M	45	VAL	5.846522	22.834	VAL
1ICC	45	VAL	5.992035	10.185	VAL
1U9U	45	VAL	6.500194	23.361	VAL
1SI8	53	VAL	6.238869	22.937	VAL
3HX9	53	VAL	10.092943	16.301	VAL
4NL5	53	VAL	5.909472	26.973	VAL
1B5M	61	VAL	6.074911	50.909	VAL
1ICC	61	VAL	5.726742	49.678	VAL
1U9U	61	VAL	6.163696	55.756	VAL
2SPL	68	VAL	5.598014	66.196	VAL
5CN5	68	VAL	5.556498	70.253	VAL
4B8N	75	VAL	6.033658	36.289	VAL
2VEB	89	VAL	5.917494	83.599	VAL
3QZZ	89	VAL	5.927268	83.889	VAL
3ZJS	89	VAL	5.790982	89.427	VAL
2O6P	119	VAL	6.176593	82.298	VAL
5KZL	124	VAL	6.607237	84.454	VAL
1SI8	125	VAL	6.016899	42.150	VAL
1IPH	127	VAL	6.256166	18.034	VAL
3VP5	131	VAL	5.568423	66.180	VAL
3VP5	148	VAL	6.888565	79.860	VAL
5O1L	152	VAL	6.293389	50.217	VAL
5O1M	152	VAL	6.250877	42.675	VAL
3QZN	161	VAL	6.290827	78.263	VAL
6A2J	175	VAL	6.202413	9.481	VAL
6A2J	182	VAL	6.679490	6.095	VAL
4CDP	192	VAL	5.600764	66.470	VAL
2J0P	195	VAL	6.307524	65.521	VAL

Table B.9: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
5O1L	197	VAL	6.648164	58.183	VAL
5O1M	197	VAL	6.631076	62.092	VAL
1IPH	199	VAL	6.294207	46.553	VAL
2IIZ	228	VAL	5.315815	34.144	VAL
2BHJ	346	VAL	6.643571	65.072	VAL
2IPS	354	VAL	6.655642	42.876	VAL
5VEU	369	VAL	6.886497	38.286	VAL
1ZVI	416	VAL	5.960795	36.384	VAL

Table B.10: HEC: All Planar Angles

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
5KPF	81	ALA	6.517051	19.673	ALA
5LFT	81	ALA	6.400723	27.359	ALA
5T8W	81	ALA	6.484127	17.792	ALA
3EAH	147	ALA	6.240842	65.476	ALA
4B2N	251	ALA	22.497312	70.131	ALA
4B2N	288	ALA	16.661485	22.769	ALA
4B2N	503	ALA	5.801904	60.592	ALA
2BC5	106	ARG	5.961420	72.519	ARG
6WZA	106	ARG	6.631682	36.834	ARG
1BBH	129	ARG	5.790808	84.690	ARG
3EAH	149	ARG	5.803314	30.280	ARG
3EAH	153	ARG	6.514542	31.482	ARG
2BC5	99	ASN	6.936196	74.457	ASN
3X15	12	CYS	6.451594	75.877	CYS
5KPF	14	CYS	6.631432	78.361	CYS
5LFT	14	CYS	6.598389	78.924	CYS
5T8W	14	CYS	6.647516	80.130	CYS
6XNK	14	CYS	6.275930	83.242	CYS
2BH5	15	CYS	6.513509	80.908	CYS
3X15	15	CYS	6.178945	60.268	CYS

Table B.10: HEC: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
5KPF	17	CYS	6.098545	57.159	CYS
5LFT	17	CYS	6.056595	55.965	CYS
5T8W	17	CYS	6.188739	57.751	CYS
6XNK	17	CYS	5.903640	67.256	CYS
1W2L	18	CYS	6.554906	79.901	CYS
2BH5	18	CYS	6.369197	56.447	CYS
1W2L	21	CYS	6.223591	50.740	CYS
2BC5	98	CYS	5.957326	62.529	CYS
6WZA	98	CYS	5.774303	65.838	CYS
2BC5	101	CYS	6.394766	89.234	CYS
6WZA	101	CYS	6.455707	88.190	CYS
1BBH	121	CYS	5.737156	69.070	CYS
1BBH	124	CYS	6.272059	73.170	CYS
3EAH	150	CYS	4.247423	47.992	CYS
4B2N	191	CYS	25.771945	51.391	CYS
4B2N	194	CYS	22.141582	46.261	CYS
6VDQ	317	CYS	6.231170	64.036	CYS
4B2N	390	CYS	6.417356	58.866	CYS
4B2N	393	CYS	6.405178	49.659	CYS
1S56	58	GLN	6.005777	46.505	GLN
1BBH	17	GLU	6.940695	44.648	GLU
4B2N	314	GLU	25.693463	52.073	GLU
3X15	24	GLY	6.352237	71.150	GLY
5KPF	29	GLY	6.052599	68.487	GLY
5LFT	29	GLY	6.048126	64.422	GLY
5T8W	29	GLY	6.153313	65.660	GLY
6XNK	29	GLY	5.786913	67.542	GLY
1W2L	31	GLY	6.565877	60.959	GLY
2BH5	36	GLY	6.126048	68.830	GLY
3EAH	152	GLY	5.627214	19.760	GLY
3X15	16	HIS	4.360557	56.339	HIS
5KPF	18	HIS	4.310334	57.026	HIS
5LFT	18	HIS	4.342999	57.434	HIS
5T8W	18	HIS	4.334295	56.673	HIS
6XNK	18	HIS	4.599701	53.280	HIS

Table B.10: HEC: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
2BH5	19	HIS	4.283790	56.825	HIS
1W2L	22	HIS	4.350769	62.051	HIS
1S56	81	HIS	4.475028	80.865	HIS
2BC5	102	HIS	4.186908	82.850	HIS
6WZA	102	HIS	4.440577	87.413	HIS
1BBH	125	HIS	4.218890	89.456	HIS
4B2N	195	HIS	20.771196	82.691	HIS
6VDQ	274	HIS	4.500421	76.928	HIS
6VDQ	313	HIS	4.120545	68.371	HIS
4B2N	394	HIS	4.305333	86.758	HIS
4B2N	641	HIS	4.333835	78.315	HIS
3X15	30	ILE	6.412845	48.363	ILE
1W2L	61	ILE	6.839545	86.856	ILE
6XNK	75	ILE	6.412701	20.309	ILE
1S56	86	ILE	5.878780	46.879	ILE
6VDQ	278	ILE	5.358791	51.036	ILE
4B2N	426	ILE	6.266877	62.886	ILE
2BC5	3	LEU	6.742954	75.724	LEU
6WZA	3	LEU	6.697674	65.670	LEU
2BC5	10	LEU	6.154091	81.531	LEU
6WZA	10	LEU	6.067786	77.978	LEU
5KPF	32	LEU	6.145036	62.380	LEU
5LFT	32	LEU	6.106815	62.454	LEU
5T8W	32	LEU	5.994375	61.079	LEU
6XNK	32	LEU	6.085909	58.350	LEU
2BH5	39	LEU	5.728784	68.293	LEU
1S56	54	LEU	5.947501	53.661	LEU
5KPF	68	LEU	6.268124	82.295	LEU
5LFT	68	LEU	6.315525	79.956	LEU
5T8W	68	LEU	6.123569	78.343	LEU
6VDQ	238	LEU	6.409586	33.875	LEU
6VDQ	277	LEU	6.506868	55.119	LEU
4B2N	506	LEU	6.039568	49.192	LEU
6XNK	79	LYS	3.938274	74.591	LYS
2BH5	100	LYS	4.313747	77.818	LYS

Table B.10: HEC: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
2BC5	7	MET	4.661903	78.629	MET
6WZA	7	MET	4.611608	76.023	MET
1BBH	19	MET	6.049470	76.193	MET
1W2L	76	MET	4.403618	74.807	MET
1S56	77	MET	6.187616	82.400	MET
5KPF	80	MET	4.692154	69.191	MET
5LFT	80	MET	4.757864	70.970	MET
5T8W	80	MET	4.693021	71.981	MET
1W2L	34	PHE	5.935685	47.542	PHE
3X15	44	PHE	6.024333	88.840	PHE
1S56	46	PHE	5.938368	40.237	PHE
2BC5	65	PHE	6.201901	7.130	PHE
6WZA	65	PHE	6.184290	8.954	PHE
5KPF	82	PHE	6.311357	54.389	PHE
5LFT	82	PHE	6.466458	54.125	PHE
5T8W	82	PHE	6.527249	55.006	PHE
2BH5	102	PHE	6.736126	35.502	PHE
4B2N	301	PHE	19.922468	12.160	PHE
4B2N	317	PHE	26.178570	38.911	PHE
3EAH	319	PHE	6.137327	43.608	PHE
6VDQ	320	PHE	6.121894	69.729	PHE
4B2N	516	PHE	6.311594	10.661	PHE
4B2N	643	PHE	5.463962	31.002	PHE
3X15	25	PRO	6.252857	53.365	PRO
5KPF	30	PRO	6.184028	58.382	PRO
5LFT	30	PRO	6.179273	58.317	PRO
5T8W	30	PRO	6.138272	60.452	PRO
6XNK	30	PRO	5.900245	78.500	PRO
1W2L	32	PRO	6.457693	61.577	PRO
2BH5	37	PRO	6.202537	54.969	PRO
5KPF	71	PRO	6.976183	22.212	PRO
5LFT	71	PRO	6.983064	24.358	PRO
5T8W	71	PRO	6.909375	23.188	PRO
1W2L	77	PRO	6.071845	79.721	PRO
4B2N	289	PRO	15.414267	83.945	PRO

Table B.10: HEC: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
4B2N	504	PRO	6.506858	70.993	PRO
1W2L	60	SER	6.470812	29.839	SER
4B2N	313	SER	24.688185	49.651	SER
6XNK	28	THR	6.983672	89.881	THR
6VDQ	309	THR	6.443589	76.554	THR
4B2N	644	THR	6.056698	22.953	THR
3EAH	144	TRP	5.647844	55.208	TRP
6VDQ	271	TRP	5.880644	62.992	TRP
4B2N	291	TRP	21.741747	22.462	TRP
3EAH	322	TRP	6.529256	31.513	TRP
1BBH	16	TYR	4.795494	83.790	TYR
1S56	33	TYR	6.252015	73.693	TYR
1BBH	58	TYR	6.554347	74.986	TYR
5KPF	67	TYR	5.922923	73.698	TYR
5LFT	67	TYR	5.919346	72.327	TYR
5T8W	67	TYR	5.858639	72.392	TYR
6XNK	67	TYR	5.613420	78.584	TYR
2BH5	79	TYR	5.535216	66.731	TYR
1W2L	80	TYR	6.249808	80.939	TYR
6VDQ	310	TYR	6.768220	38.505	TYR
1W2L	75	VAL	6.753821	70.180	VAL
1S56	80	VAL	6.205932	89.256	VAL
2BH5	80	VAL	6.887770	66.644	VAL
6XNK	83	VAL	6.004096	49.708	VAL
1S56	94	VAL	6.626107	47.118	VAL
1S56	126	VAL	6.029592	82.902	VAL
3EAH	151	VAL	6.103944	46.478	VAL
4B2N	527	VAL	6.028491	21.483	VAL

Table B.11: SRM: All Planar Angles

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
1ZJ8	468	ALA	6.774896	67.235	ALA
3B0G	486	ALA	6.469408	53.215	ALA
3VKP	486	ALA	6.471195	63.024	ALA
3VLX	486	ALA	6.481752	63.686	ALA
3VLY	486	ALA	6.503895	62.464	ALA
3VLZ	486	ALA	6.507235	52.788	ALA
5H8V	545	ALA	6.528336	65.454	ALA
2AOP	83	ARG	5.905472	47.714	ARG
1ZJ8	97	ARG	5.632921	36.797	ARG
2AKJ	109	ARG	5.624044	45.808	ARG
3B0G	109	ARG	5.714505	49.905	ARG
3VKP	109	ARG	5.727950	45.457	ARG
3VLX	109	ARG	5.657293	44.382	ARG
3VLY	109	ARG	5.670401	44.269	ARG
3VLZ	109	ARG	5.666461	48.083	ARG
5H8V	124	ARG	5.731236	44.003	ARG
2AOP	153	ARG	6.898322	85.374	ARG
1ZJ8	166	ARG	6.411696	86.955	ARG
2AKJ	179	ARG	6.270969	87.072	ARG
3B0G	179	ARG	6.332302	75.820	ARG
3VKP	179	ARG	6.261289	85.962	ARG
3VLX	179	ARG	6.332845	87.012	ARG
3VLY	179	ARG	6.349458	86.279	ARG
3VLZ	179	ARG	6.432708	75.861	ARG
5H8V	193	ARG	6.748373	86.970	ARG
2AOP	116	ASN	6.627004	77.523	ASN
1ZJ8	465	ASN	6.589731	74.338	ASN
2AOP	481	ASN	6.568014	76.265	ASN
3B0G	483	ASN	6.105308	61.801	ASN
3VKP	483	ASN	6.093849	72.638	ASN
3VLX	483	ASN	6.149563	73.596	ASN
3VLY	483	ASN	6.199685	72.914	ASN
3VLZ	483	ASN	6.172324	60.497	ASN
2AKJ	484	ASN	6.180565	72.711	ASN
5H8V	542	ASN	6.517505	79.233	ASN

Table B.11: SRM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
1ZJ8	129	ASP	6.873987	67.150	ASP
1ZJ8	467	CYS	4.642760	87.220	CYS
2AOP	483	CYS	4.593058	85.931	CYS
3B0G	485	CYS	4.334547	73.017	CYS
3VKP	485	CYS	4.338921	84.887	CYS
3VLX	485	CYS	4.333556	85.502	CYS
3VLY	485	CYS	4.349260	84.134	CYS
3VLZ	485	CYS	4.361247	73.065	CYS
2AKJ	486	CYS	4.400598	86.391	CYS
5H8V	494	CYS	6.918908	18.748	CYS
5H8V	544	CYS	4.294361	85.621	CYS
2AOP	121	GLN	6.832109	25.136	GLN
1ZJ8	134	GLN	6.870508	22.173	GLN
5H8V	161	GLN	6.725078	29.150	GLN
2AOP	482	GLY	6.644058	75.745	GLY
2AOP	484	GLY	6.751562	83.876	GLY
2AKJ	487	GLY	6.536313	79.167	GLY
5H8V	543	GLY	6.487994	78.451	GLY
1ZJ8	207	LYS	5.279599	51.736	LYS
1ZJ8	209	LYS	5.254105	61.416	LYS
2AOP	215	LYS	5.521547	41.259	LYS
2AOP	217	LYS	5.485034	57.432	LYS
2AKJ	224	LYS	5.292960	53.525	LYS
3B0G	224	LYS	5.579947	59.557	LYS
3VKP	224	LYS	5.500133	56.004	LYS
3VLX	224	LYS	5.605021	56.372	LYS
3VLY	224	LYS	5.637976	59.364	LYS
3VLZ	224	LYS	5.601385	52.886	LYS
3VLY	226	LYS	5.485627	52.123	LYS
3VLZ	226	LYS	5.641233	47.713	LYS
5H8V	276	LYS	5.805329	50.247	LYS
5H8V	278	LYS	5.495851	53.934	LYS
1ZJ8	466	SER	6.539429	45.045	SER
2AKJ	485	SER	6.504302	77.035	SER
2AKJ	142	THR	6.814343	68.034	THR

Table B.11: SRM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
3B0G	142	THR	6.442796	66.277	THR
3VKP	142	THR	6.428882	73.086	THR
3VLX	142	THR	6.455248	73.866	THR
3VLY	142	THR	6.452740	72.255	THR
3VLZ	142	THR	6.394057	69.555	THR
5H8V	156	THR	6.490994	74.765	THR
3B0G	484	THR	6.402854	34.005	THR
3VKP	484	THR	6.412766	38.529	THR
3VLX	484	THR	6.401875	38.523	THR
3VLY	484	THR	6.414362	37.480	THR
3VLZ	484	THR	6.437540	35.092	THR
1ZJ8	69	TYR	6.963349	17.492	TYR
5H8V	106	TYR	6.992106	27.541	TYR

Table B.12: VERDOHEME: All Planar Angles

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
2ZVU	28	ALA	6.962159	60.211	ALA
3MOO	136	ASP	6.778611	59.636	ASP
2ZVU	140	ASP	6.674210	53.858	ASP
3MOO	24	GLU	6.275511	34.237	GLU
2ZVU	29	GLU	6.221641	12.615	GLU
3MOO	135	GLY	5.288496	66.356	GLY
2ZVU	139	GLY	5.265696	66.938	GLY
3MOO	139	GLY	5.369017	35.165	GLY
3MOO	140	GLY	6.027517	69.523	GLY
2ZVU	143	GLY	5.436145	32.937	GLY
2ZVU	144	GLY	5.902504	68.684	GLY
3MOO	20	HIS	4.614778	65.389	HIS
2ZVU	25	HIS	4.603252	70.790	HIS
3MOO	134	LEU	6.100073	27.652	LEU

Table B.12: VERDOHEME: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
2ZVU	138	LEU	6.249768	37.499	LEU
3MOO	201	PHE	5.958999	31.400	PHE
2ZVU	207	PHE	6.037412	29.522	PHE
3MOO	138	SER	5.886820	52.337	SER
2ZVU	142	SER	6.048311	54.957	SER
2ZVU	135	THR	6.765195	89.631	THR
3MOO	131	VAL	6.796515	89.945	VAL
1TWN	140	ASP	6.273979	75.887	ASP
1TWR	140	ASP	6.553790	73.555	ASP
1TWN	29	GLU	6.123574	35.411	GLU
1TWR	29	GLU	6.517157	50.624	GLU
1TWN	139	GLY	5.092800	37.268	GLY
1TWR	139	GLY	5.369385	36.457	GLY
1TWN	143	GLY	5.231213	20.583	GLY
1TWR	143	GLY	5.836559	26.276	GLY
1TWN	144	GLY	6.024952	48.406	GLY
1TWN	25	HIS	4.673370	82.070	HIS
1TWR	25	HIS	4.786588	75.802	HIS
1TWN	138	LEU	6.399559	8.072	LEU
1TWR	138	LEU	6.579770	2.665	LEU
1TWN	207	PHE	6.263716	53.897	PHE
1TWR	207	PHE	6.447849	51.949	PHE
1TWN	142	SER	6.035867	26.649	SER
1TWR	142	SER	6.195017	40.009	SER
1TWN	135	THR	6.865192	71.849	THR

B.4 Planar Angles of Closest Residues

Table B.13: HEM: Planar Angles of Closest Residues

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
1B2V	75	TYR	4.251885	39.160	TYR
1B2V	32	HIS	4.667618	51.415	HIS
1B2V	83	HIS	5.366599	56.778	HIS
1B5M	63	HIS	4.211990	71.272	HIS
1B5M	39	HIS	4.456809	87.693	HIS
1B5M	41	GLY	5.388127	72.708	GLY
1DK0	75	TYR	4.346840	40.042	TYR
1DK0	32	HIS	4.556145	48.497	HIS
1DK0	83	HIS	5.314133	62.320	HIS
1DKH	75	TYR	4.792830	45.976	TYR
1DKH	32	HIS	5.099382	50.187	HIS
1DKH	83	HIS	5.223800	43.522	HIS
1ICC	63	HIS	4.451283	57.814	HIS
1ICC	39	HIS	4.542187	78.752	HIS
1ICC	41	GLY	5.723853	72.752	GLY
1IPH	415	TYR	4.218561	62.200	TYR
1IPH	411	ARG	5.321024	79.235	ARG
1IPH	128	HIS	5.713777	33.997	HIS
1N45	25	HIS	4.545004	69.116	HIS
1N45	139	GLY	5.251379	58.119	GLY
1N45	143	GLY	5.882948	37.778	GLY
1P3T	23	HIS	4.573926	67.542	HIS
1P3T	120	GLY	4.843774	41.129	GLY
1P3T	117	SER	5.531584	72.173	SER
1QHU	265	HIS	4.200094	83.910	HIS
1QHU	213	HIS	4.734866	79.430	HIS
1QHU	267	TRP	5.987630	76.604	TRP
1QJS	266	HIS	4.484379	82.026	HIS
1QJS	213	HIS	4.696712	82.802	HIS
1QJS	171	TRP	6.211700	40.663	TRP
1SI8	337	TYR	3.976560	58.339	TYR
1SI8	333	ARG	5.247624	87.335	ARG
1SI8	140	PHE	5.575451	44.222	PHE
1SY2	59	HIS	4.045387	85.351	HIS
1SY2	40	TYR	5.887937	30.456	TYR

Table B.13: HEM: Planar Angles of Closest Residues *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
1SY2	123	LEU	5.902915	71.098	LEU
1U9U	63	HIS	4.417873	66.393	HIS
1U9U	39	HIS	4.589294	80.451	HIS
1U9U	41	GLY	5.723510	83.944	GLY
1VGI	25	HIS	4.646180	72.142	HIS
1VGI	139	GLY	5.155470	60.437	GLY
1VGI	143	GLY	5.279720	32.760	GLY
1ZVI	415	CYS	4.181834	46.871	CYS
1ZVI	417	GLY	5.404983	24.763	GLY
1ZVI	409	TRP	5.660275	56.622	TRP
2BHJ	194	CYS	4.487497	52.816	CYS
2BHJ	196	GLY	5.667103	19.625	GLY
2BHJ	193	ARG	5.745098	22.913	ARG
2CJ0	29	CYS	4.390905	47.217	CYS
2CJ0	31	ALA	5.440871	54.576	ALA
2CJ0	183	GLU	5.716050	77.664	GLU
2CN4	75	TYR	4.345054	45.523	TYR
2CN4	83	HIS	5.251875	61.039	HIS
2CN4	140	MET	5.816277	79.067	MET
2CPO	29	CYS	4.443549	49.291	CYS
2CPO	31	ALA	5.505123	50.842	ALA
2CPO	183	GLU	5.799506	78.548	GLU
2E2Y	93	HIS	4.514535	86.534	HIS
2E2Y	68	ILE	5.517060	80.623	ILE
2E2Y	43	TRP	5.845537	63.663	TRP
2FC2	62	CYS	4.482879	54.005	CYS
2FC2	56	TRP	5.737975	58.198	TRP
2FC2	64	GLY	5.882725	21.989	GLY
2IIZ	224	HIS	4.533607	61.464	HIS
2IIZ	242	ARG	5.236889	71.798	ARG
2IIZ	228	VAL	5.315815	34.144	VAL
2IPS	351	HIS	4.125792	28.391	HIS
2IPS	433	LEU	5.458537	63.062	LEU
2IPS	108	ASP	5.870986	78.247	ASP
2J0P	196	HIS	4.310325	75.104	HIS

Table B.13: HEM: Planar Angles of Closest Residues *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
2J0P	102	ARG	5.002395	83.046	ARG
2J0P	246	PHE	6.155004	71.919	PHE
2J18	29	CYS	4.359887	47.527	CYS
2J18	31	ALA	5.457126	52.882	ALA
2J18	183	GLU	5.722472	78.531	GLU
2O6P	132	TYR	4.055037	56.191	TYR
2O6P	136	TYR	5.148558	86.464	TYR
2O6P	48	ILE	5.365972	44.466	ILE
2Q6N	436	CYS	4.305637	40.993	CYS
2Q6N	438	GLY	5.615678	28.366	GLY
2Q6N	298	ALA	5.672036	28.414	ALA
2R7A	67	TYR	4.159993	73.259	TYR
2R7A	169	ALA	5.223004	39.141	ALA
2R7A	257	LEU	5.559331	26.488	LEU
2SPL	93	HIS	4.578545	88.954	HIS
2SPL	68	VAL	5.598014	66.196	VAL
2SPL	43	PHE	5.815167	43.358	PHE
2VEB	120	HIS	4.471709	79.839	HIS
2VEB	185	TRP	5.717992	82.552	TRP
2VEB	93	PHE	5.810118	22.043	PHE
3HX9	75	HIS	4.195649	50.709	HIS
3HX9	71	ALA	6.230664	24.118	ALA
3HX9	66	TRP	7.852796	51.391	TRP
3MVF	59	HIS	4.066882	87.977	HIS
3MVF	42	ALA	5.827660	37.714	ALA
3MVF	123	LEU	5.891492	77.839	LEU
3QZN	83	HIS	4.660500	67.495	HIS
3QZN	170	TYR	5.718488	72.518	TYR
3QZN	159	ILE	5.866079	87.212	ILE
3QZZ	120	HIS	4.599066	74.693	HIS
3QZZ	89	VAL	5.927268	83.889	VAL
3QZZ	93	PHE	6.033470	11.038	PHE
3SIK	136	TYR	4.260470	52.942	TYR
3SIK	140	TYR	5.120136	63.829	TYR
3SIK	54	ARG	6.090293	58.962	ARG

Table B.13: HEM: Planar Angles of Closest Residues *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
3TGC	59	HIS	4.100823	87.207	HIS
3TGC	123	LEU	5.908675	73.018	LEU
3TGC	40	TYR	5.967215	29.632	TYR
3VP5	149	HIS	4.350835	49.264	HIS
3VP5	72	HIS	4.371971	45.918	HIS
3VP5	131	VAL	5.568423	66.180	VAL
3ZJS	120	HIS	4.427156	73.923	HIS
3ZJS	89	VAL	5.790982	89.427	VAL
3ZJS	93	PHE	5.922481	16.833	PHE
4B8N	71	HIS	4.416116	70.933	HIS
4B8N	48	HIS	4.479396	87.524	HIS
4B8N	50	GLY	5.464969	87.471	GLY
4CDP	193	HIS	4.417630	74.031	HIS
4CDP	100	ARG	5.360373	82.404	ARG
4CDP	192	VAL	5.600764	66.470	VAL
4I3Q	442	CYS	4.085782	34.781	CYS
4I3Q	444	GLY	5.222394	22.218	GLY
4I3Q	305	ALA	5.305272	55.811	ALA
4JET	75	TYR	4.420106	47.089	TYR
4JET	81	HIS	5.381133	54.183	HIS
4JET	40	ARG	5.660400	8.293	ARG
4MF9	209	HIS	4.606487	63.203	HIS
4MF9	112	ARG	5.056393	85.919	ARG
4MF9	259	PHE	5.680334	67.502	PHE
4MYP	280	TYR	4.465249	56.836	TYR
4MYP	289	TYR	5.900895	20.187	TYR
4MYP	293	ALA	6.207799	64.118	ALA
4NL5	75	HIS	4.473936	46.347	HIS
4NL5	7	ASN	5.402231	60.999	ASN
4NL5	23	PHE	5.580423	79.989	PHE
4UZV	106	HIS	4.502311	79.507	HIS
4UZV	119	PHE	5.820671	52.586	PHE
4UZV	111	ILE	5.897899	46.982	ILE
4XZD	75	TYR	4.329954	46.839	TYR
4XZD	81	HIS	5.263108	67.684	HIS

Table B.13: HEM: Planar Angles of Closest Residues *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
4XZD	40	ARG	5.892195	23.940	ARG
4Y1Q	81	HIS	5.294289	61.474	HIS
4Y1Q	40	ARG	5.725205	11.586	ARG
4Y1Q	147	MET	6.115760	72.668	MET
5CN5	93	HIS	4.575365	82.799	HIS
5CN5	68	VAL	5.556498	70.253	VAL
5CN5	64	HIS	5.804727	84.840	HIS
5GJ3	239	TYR	4.170326	62.993	TYR
5GJ3	241	ARG	5.542517	89.231	ARG
5GJ3	140	TYR	7.520130	58.494	TYR
5KZL	15	HIS	4.819650	59.949	HIS
5KZL	128	GLY	5.130966	70.591	GLY
5KZL	132	GLY	5.705062	50.430	GLY
5O1L	198	HIS	4.305405	66.467	HIS
5O1L	171	LEU	5.743071	78.726	LEU
5O1L	222	ILE	6.024951	24.897	ILE
5O1M	198	HIS	4.392715	64.463	HIS
5O1M	167	LYS	5.125712	80.116	LYS
5O1M	222	ILE	6.241067	30.392	ILE
5VEU	441	CYS	4.349464	42.614	CYS
5VEU	443	GLY	5.482822	27.362	GLY
5VEU	309	THR	5.895842	31.467	THR
6A2J	216	HIS	4.601722	63.468	HIS
6A2J	278	HIS	4.655598	63.931	HIS
6A2J	179	GLY	5.548597	36.551	GLY
7C74	351	HIS	4.494179	25.953	HIS
7C74	433	LEU	5.275537	56.669	LEU
7C74	105	GLN	5.667218	84.879	GLN
7DMR	351	HIS	4.201640	31.126	HIS
7DMR	433	LEU	5.225161	71.791	LEU
7DMR	105	GLN	5.517249	82.031	GLN

Table B.14: HEC: Planar Angles of Closest Residues

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
1BBH	125	HIS	4.218890	89.456	HIS
1BBH	16	TYR	4.795494	83.790	TYR
1BBH	121	CYS	5.737156	69.070	CYS
1S56	81	HIS	4.475028	80.865	HIS
1S56	86	ILE	5.878780	46.879	ILE
1S56	46	PHE	5.938368	40.237	PHE
1W2L	22	HIS	4.350769	62.051	HIS
1W2L	76	MET	4.403618	74.807	MET
1W2L	34	PHE	5.935685	47.542	PHE
2BC5	102	HIS	4.186908	82.850	HIS
2BC5	7	MET	4.661903	78.629	MET
2BC5	98	CYS	5.957326	62.529	CYS
2BH5	19	HIS	4.283790	56.825	HIS
2BH5	100	LYS	4.313747	77.818	LYS
2BH5	79	TYR	5.535216	66.731	TYR
3EAH	150	CYS	4.247423	47.992	CYS
3EAH	152	GLY	5.627214	19.760	GLY
3EAH	144	TRP	5.647844	55.208	TRP
3X15	16	HIS	4.360557	56.339	HIS
3X15	44	PHE	6.024333	88.840	PHE
3X15	15	CYS	6.178945	60.268	CYS
4B2N	394	HIS	4.305333	86.758	HIS
4B2N	641	HIS	4.333835	78.315	HIS
4B2N	643	PHE	5.463962	31.002	PHE
5KPF	18	HIS	4.310334	57.026	HIS
5KPF	80	MET	4.692154	69.191	MET
5KPF	67	TYR	5.922923	73.698	TYR
5LFT	18	HIS	4.342999	57.434	HIS
5LFT	80	MET	4.757864	70.970	MET
5LFT	67	TYR	5.919346	72.327	TYR
5T8W	18	HIS	4.334295	56.673	HIS
5T8W	80	MET	4.693021	71.981	MET
5T8W	67	TYR	5.858639	72.392	TYR
6VDQ	313	HIS	4.120545	68.371	HIS
6VDQ	274	HIS	4.500421	76.928	HIS

Table B.14: HEC: Planar Angles of Closest Residues *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
6VDQ	278	ILE	5.358791	51.036	ILE
6WZA	102	HIS	4.440577	87.413	HIS
6WZA	7	MET	4.611608	76.023	MET
6WZA	98	CYS	5.774303	65.838	CYS
6XNK	79	LYS	3.938274	74.591	LYS
6XNK	18	HIS	4.599701	53.280	HIS
6XNK	67	TYR	5.613420	78.584	TYR

Table B.15: SRM: Planar Angles of Closest Residues

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
1ZJ8	467	CYS	4.642760	87.220	CYS
1ZJ8	209	LYS	5.254105	61.416	LYS
1ZJ8	207	LYS	5.279599	51.736	LYS
2AKJ	486	CYS	4.400598	86.391	CYS
2AKJ	224	LYS	5.292960	53.525	LYS
2AKJ	109	ARG	5.624044	45.808	ARG
2AOP	483	CYS	4.593058	85.931	CYS
2AOP	217	LYS	5.485034	57.432	LYS
2AOP	215	LYS	5.521547	41.259	LYS
3B0G	485	CYS	4.334547	73.017	CYS
3B0G	224	LYS	5.579947	59.557	LYS
3B0G	109	ARG	5.714505	49.905	ARG
3VKP	485	CYS	4.338921	84.887	CYS
3VKP	224	LYS	5.500133	56.004	LYS
3VKP	109	ARG	5.727950	45.457	ARG
3VLX	485	CYS	4.333556	85.502	CYS
3VLX	224	LYS	5.605021	56.372	LYS
3VLX	109	ARG	5.657293	44.382	ARG
3VLY	485	CYS	4.349260	84.134	CYS
3VLY	226	LYS	5.485627	52.123	LYS

Table B.15: SRM: Planar Angles of Closest Residues *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
3VLY	224	LYS	5.637976	59.364	LYS
3VLZ	485	CYS	4.361247	73.065	CYS
3VLZ	224	LYS	5.601385	52.886	LYS
3VLZ	226	LYS	5.641233	47.713	LYS
5H8V	544	CYS	4.294361	85.621	CYS
5H8V	278	LYS	5.495851	53.934	LYS
5H8V	124	ARG	5.731236	44.003	ARG

Table B.16: VERDOHEME: Planar Angles of Closest Residues

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
2ZVU	25	HIS	4.603252	70.790	HIS
2ZVU	139	GLY	5.265696	66.938	GLY
2ZVU	143	GLY	5.436145	32.937	GLY
3MOO	20	HIS	4.614778	65.389	HIS
3MOO	135	GLY	5.288496	66.356	GLY
3MOO	139	GLY	5.369017	35.165	GLY
1TWN	25	HIS	4.673370	82.070	HIS
1TWN	139	GLY	5.092800	37.268	GLY
1TWN	143	GLY	5.231213	20.583	GLY
1TWR	25	HIS	4.786588	75.802	HIS
1TWR	139	GLY	5.369385	36.457	GLY
1TWR	143	GLY	5.836559	26.276	GLY

B.5 All CA-CB-Fe Angles

Table B.17: HEM: All CA-CB-Fe Angles

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
1N45	28	ALA	6.981230	ALA	133.1800
2CJ0	31	ALA	5.440871	ALA	114.8710
2CPO	31	ALA	5.505123	ALA	115.0400
2J18	31	ALA	5.457126	ALA	114.2550
1SY2	42	ALA	6.006055	ALA	148.0360
3MVF	42	ALA	5.827660	ALA	147.3790
3TGC	42	ALA	6.033598	ALA	151.3290
2O6P	49	ALA	6.356063	ALA	69.6260
4B8N	54	ALA	6.390793	ALA	135.4860
1B5M	67	ALA	5.797296	ALA	143.9450
1ICC	67	ALA	6.085233	ALA	131.3420
1U9U	67	ALA	6.016697	ALA	136.6100
2CJ0	71	ALA	6.531120	ALA	140.1920
2CPO	71	ALA	6.539227	ALA	137.2830
2J18	71	ALA	6.477348	ALA	139.0360
4NL5	71	ALA	6.805378	ALA	99.7605
4Y1Q	75	ALA	6.722226	ALA	130.5910
1P3T	121	ALA	6.382367	ALA	48.9641
3SIK	138	ALA	6.231014	ALA	159.2210
2R7A	169	ALA	5.223004	ALA	132.6020
6A2J	180	ALA	6.687029	ALA	43.4302
2BHJ	191	ALA	6.261711	ALA	163.9660
6A2J	220	ALA	5.986896	ALA	140.0610
6A2J	259	ALA	6.937825	ALA	40.3063
4MYP	282	ALA	6.581195	ALA	153.2720
4MYP	293	ALA	6.207799	ALA	133.2580
2Q6N	298	ALA	5.672036	ALA	129.8410
4I3Q	305	ALA	5.305272	ALA	115.6050
5VEU	305	ALA	6.219660	ALA	130.5820
1ZVI	412	ALA	6.481380	ALA	147.8760
2Q6N	442	ALA	6.935846	ALA	147.6550
5VEU	447	ALA	6.667315	ALA	149.4040
4I3Q	448	ALA	6.441232	ALA	146.6870
4JET	40	ARG	5.660400	ARG	117.6700
4XZD	40	ARG	5.892195	ARG	118.8830

Table B.17: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
4Y1Q	40	ARG	5.725205	ARG	121.1480
3SIK	54	ARG	6.090293	ARG	163.0460
2FC2	61	ARG	6.072553	ARG	76.2562
2FC2	65	ARG	6.459491	ARG	70.9521
4CDP	100	ARG	5.360373	ARG	139.0430
2J0P	102	ARG	5.002395	ARG	139.6090
4UZV	105	ARG	6.689489	ARG	101.6930
4MF9	112	ARG	5.056393	ARG	134.9890
4JET	144	ARG	6.239587	ARG	94.9228
4XZD	144	ARG	6.335714	ARG	98.1313
4Y1Q	144	ARG	6.425880	ARG	98.5684
2BHJ	193	ARG	5.745098	ARG	61.6429
2BHJ	197	ARG	6.221230	ARG	67.6390
4I3Q	212	ARG	6.392849	ARG	133.1990
1QHU	214	ARG	6.588734	ARG	137.0270
1QJS	214	ARG	6.249190	ARG	70.2144
6A2J	217	ARG	6.781589	ARG	54.8831
2IIZ	242	ARG	5.236889	ARG	162.0190
1SI8	333	ARG	5.247624	ARG	116.1170
2IPS	348	ARG	6.336679	ARG	87.8395
7C74	348	ARG	6.274279	ARG	78.0301
7DMR	348	ARG	6.250958	ARG	82.5509
1IPH	411	ARG	5.321024	ARG	108.2630
1ZVI	414	ARG	5.799426	ARG	71.6516
1ZVI	418	ARG	6.259544	ARG	69.7795
4NL5	7	ASN	5.402231	ASN	170.5520
1B2V	41	ASN	6.894251	ASN	79.4068
1DK0	41	ASN	6.870425	ASN	80.6960
1P3T	118	ASN	6.625279	ASN	26.9658
1SI8	127	ASN	6.666708	ASN	103.3680
1IPH	201	ASN	6.396844	ASN	101.2860
2BHJ	364	ASN	6.955669	ASN	23.4362
2IPS	437	ASN	6.276979	ASN	111.3700
7C74	437	ASN	6.653391	ASN	112.3740
7DMR	437	ASN	6.591349	ASN	110.5710

Table B.17: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
5VEU	440	ASN	6.408862	ASN	56.4019
4I3Q	441	ASN	6.139159	ASN	60.3712
1P3T	27	ASP	6.267807	ASP	103.4810
2E2Y	64	ASP	6.865050	ASP	101.7770
2IPS	108	ASP	5.870986	ASP	152.6010
7C74	108	ASP	6.017401	ASP	160.5440
7DMR	108	ASP	6.266021	ASP	151.6240
1N45	140	ASP	6.389011	ASP	35.7360
1VGI	140	ASP	6.566393	ASP	22.5121
2IIZ	151	ASP	5.861207	ASP	97.0879
4CDP	191	ASP	6.789427	ASP	101.3160
2J0P	194	ASP	6.862392	ASP	107.8210
1QHU	203	ASP	6.920576	ASP	76.4671
1QJS	203	ASP	6.878437	ASP	70.4888
2IIZ	284	ASP	6.598336	ASP	144.2720
2CJ0	29	CYS	4.390905	CYS	117.5660
2CPO	29	CYS	4.443549	CYS	118.1890
2J18	29	CYS	4.359887	CYS	118.4250
2FC2	62	CYS	4.482879	CYS	112.5820
1P3T	113	CYS	6.881310	CYS	62.2220
2BHJ	194	CYS	4.487497	CYS	118.0500
1ZVI	415	CYS	4.181834	CYS	112.7440
2Q6N	436	CYS	4.305637	CYS	109.8240
5VEU	441	CYS	4.349464	CYS	106.7690
4I3Q	442	CYS	4.085782	CYS	103.9950
2IPS	105	GLN	5.981590	GLN	100.5170
7C74	105	GLN	5.667218	GLN	97.8161
7DMR	105	GLN	5.517249	GLN	100.6130
2R7A	253	GLN	6.081153	GLN	123.5700
6A2J	258	GLN	5.803666	GLN	91.0438
4MYP	292	GLN	6.537566	GLN	16.1591
1N45	29	GLU	6.277510	GLU	93.8698
1VGI	29	GLU	6.279863	GLU	118.3990
5O1L	148	GLU	6.440638	GLU	94.5791
2CJ0	183	GLU	5.716050	GLU	106.0810

Table B.17: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
2CPO	183	GLU	5.799506	GLU	105.9460
2J18	183	GLU	5.722472	GLU	107.1960
1QHU	225	GLU	6.177350	GLU	167.2860
1QJS	226	GLU	6.465511	GLU	155.6740
2IPS	258	GLU	6.388898	GLU	174.0360
7C74	258	GLU	6.258582	GLU	160.0830
7DMR	258	GLU	6.172262	GLU	155.5410
2Q6N	439	GLU	6.270464	GLU	58.8909
1ZVI	592	GLU	6.601349	GLU	140.0500
1P3T	23	HIS	4.573926	HIS	111.7580
1N45	25	HIS	4.545004	HIS	112.7600
1VGI	25	HIS	4.646180	HIS	113.1630
1B2V	32	HIS	4.667618	HIS	116.3150
1DK0	32	HIS	4.556145	HIS	116.4470
1DKH	32	HIS	5.099382	HIS	121.3750
1B5M	39	HIS	4.456809	HIS	101.8130
1ICC	39	HIS	4.542187	HIS	101.5070
1U9U	39	HIS	4.589294	HIS	102.2750
4B8N	48	HIS	4.479396	HIS	104.9040
1SI8	54	HIS	5.688888	HIS	131.6120
1SY2	59	HIS	4.045387	HIS	126.3700
3MVF	59	HIS	4.066882	HIS	126.0770
3TGC	59	HIS	4.100823	HIS	124.3700
1B5M	63	HIS	4.211990	HIS	125.8380
1ICC	63	HIS	4.451283	HIS	114.1290
1U9U	63	HIS	4.417873	HIS	116.0130
2SPL	64	HIS	5.889080	HIS	103.2250
5CN5	64	HIS	5.804727	HIS	107.1420
4B8N	71	HIS	4.416116	HIS	119.3920
3VP5	72	HIS	4.371971	HIS	101.6570
4NL5	75	HIS	4.473936	HIS	117.7090
4JET	81	HIS	5.381133	HIS	121.2740
4XZD	81	HIS	5.263108	HIS	114.4420
4Y1Q	81	HIS	5.294289	HIS	126.8310
1B2V	83	HIS	5.366599	HIS	102.9160

Table B.17: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
1DK0	83	HIS	5.314133	HIS	102.7520
1DKH	83	HIS	5.223800	HIS	122.9600
2CN4	83	HIS	5.251875	HIS	107.5140
2E2Y	93	HIS	4.514535	HIS	114.4980
2SPL	93	HIS	4.578545	HIS	112.4730
5CN5	93	HIS	4.575365	HIS	113.1870
2E2Y	97	HIS	5.917056	HIS	177.1860
2SPL	97	HIS	5.997752	HIS	176.0860
5CN5	97	HIS	5.966408	HIS	177.3970
4UZV	106	HIS	4.502311	HIS	110.2430
2IPS	109	HIS	5.924623	HIS	93.6174
7C74	109	HIS	5.952700	HIS	93.3571
7DMR	109	HIS	5.699226	HIS	93.5665
2VEB	120	HIS	4.471709	HIS	110.4880
3QZZ	120	HIS	4.599066	HIS	109.3460
3ZJS	120	HIS	4.427156	HIS	110.7000
1IPH	128	HIS	5.713777	HIS	129.2180
2O6P	134	HIS	6.496593	HIS	146.7790
3VP5	149	HIS	4.350835	HIS	100.8200
4CDP	193	HIS	4.417630	HIS	109.7720
2J0P	196	HIS	4.310325	HIS	111.1620
5O1L	198	HIS	4.305405	HIS	102.4410
5O1M	198	HIS	4.392715	HIS	100.3070
4MF9	209	HIS	4.606487	HIS	108.6490
1QHU	213	HIS	4.734866	HIS	114.5350
1QJS	213	HIS	4.696712	HIS	122.0930
6A2J	216	HIS	4.601722	HIS	122.2890
1QHU	222	HIS	6.740296	HIS	173.7070
2IIZ	224	HIS	4.533607	HIS	124.3380
1QHU	265	HIS	4.200094	HIS	121.1810
1QJS	266	HIS	4.484379	HIS	120.9930
6A2J	278	HIS	4.655598	HIS	124.6210
2IPS	351	HIS	4.125792	HIS	94.9759
7C74	351	HIS	4.494179	HIS	92.7950
7DMR	351	HIS	4.201640	HIS	96.7615

Table B.17: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
4NL5	9	ILE	5.756873	ILE	125.9250
4JET	30	ILE	6.988601	ILE	147.5590
2O6P	48	ILE	5.365972	ILE	141.3220
4B8N	55	ILE	5.758462	ILE	101.7060
2FC2	63	ILE	6.106378	ILE	55.1533
2E2Y	68	ILE	5.517060	ILE	97.7283
3VP5	71	ILE	6.407016	ILE	105.2440
2E2Y	99	ILE	6.130795	ILE	160.7990
2SPL	99	ILE	6.223033	ILE	157.6520
5CN5	99	ILE	6.410362	ILE	160.0190
2E2Y	107	ILE	6.704700	ILE	171.6940
2SPL	107	ILE	6.505472	ILE	170.3470
5CN5	107	ILE	6.767432	ILE	172.1900
4UZV	111	ILE	5.897899	ILE	140.3930
2Q6N	114	ILE	6.560571	ILE	116.0170
2VEB	116	ILE	6.573571	ILE	101.7820
3QZZ	116	ILE	6.472356	ILE	100.9480
3ZJS	116	ILE	6.518950	ILE	103.0000
2O6P	121	ILE	6.852081	ILE	132.2050
3SIK	129	ILE	6.189129	ILE	165.5190
3SIK	131	ILE	6.481115	ILE	134.1420
2VEB	137	ILE	6.361213	ILE	179.1050
3QZZ	137	ILE	6.393964	ILE	177.4290
3ZJS	137	ILE	6.315026	ILE	177.5600
2BHJ	195	ILE	6.216303	ILE	54.9628
2FC2	214	ILE	6.545905	ILE	136.6930
5O1L	222	ILE	6.024951	ILE	133.4090
5O1M	222	ILE	6.241067	ILE	136.2240
2IIZ	225	ILE	6.430481	ILE	59.8660
5O1L	227	ILE	6.973430	ILE	87.0131
4CDP	252	ILE	6.178209	ILE	160.7780
2J0P	255	ILE	6.197370	ILE	154.1260
6A2J	265	ILE	6.271826	ILE	147.7330
4MF9	268	ILE	6.092502	ILE	155.0200
2Q6N	363	ILE	6.794813	ILE	150.8430

Table B.17: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
2Q6N	435	ILE	6.531691	ILE	50.7026
5VEU	442	ILE	6.119535	ILE	59.4678
4I3Q	443	ILE	5.985023	ILE	55.5209
2CJ0	32	LEU	5.757197	LEU	97.6039
2CPO	32	LEU	5.913058	LEU	99.3621
2J18	32	LEU	5.760472	LEU	96.2823
1B5M	46	LEU	5.848737	LEU	104.5310
1ICC	46	LEU	5.941384	LEU	99.3266
1U9U	46	LEU	5.958763	LEU	99.9911
1SY2	57	LEU	6.145372	LEU	142.4070
3MVF	57	LEU	6.242544	LEU	143.0050
3TGC	57	LEU	6.147624	LEU	140.8920
4B8N	70	LEU	6.456250	LEU	123.0540
1B2V	77	LEU	6.429830	LEU	57.1497
1DK0	77	LEU	6.502332	LEU	58.1793
1DKH	77	LEU	6.345588	LEU	66.1552
2CN4	77	LEU	6.548785	LEU	53.5337
4UZV	79	LEU	6.352126	LEU	105.2350
2E2Y	89	LEU	6.167984	LEU	89.7887
2SPL	89	LEU	6.446644	LEU	83.4261
5CN5	89	LEU	6.607510	LEU	97.7142
4CDP	90	LEU	6.499175	LEU	152.7650
4UZV	102	LEU	6.801707	LEU	85.2040
2E2Y	104	LEU	6.384225	LEU	87.1682
2SPL	104	LEU	6.518599	LEU	83.9530
5CN5	104	LEU	6.517400	LEU	86.5002
1P3T	119	LEU	6.709401	LEU	90.3174
1SY2	123	LEU	5.902915	LEU	147.6300
3MVF	123	LEU	5.891492	LEU	147.9850
3TGC	123	LEU	5.908675	LEU	148.3100
1SY2	133	LEU	6.241713	LEU	171.7810
3MVF	133	LEU	6.341681	LEU	176.8730
3TGC	133	LEU	6.315080	LEU	175.4300
1N45	138	LEU	6.717099	LEU	68.2659
1VGI	138	LEU	6.110494	LEU	81.0454

Table B.17: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
2VEB	142	LEU	6.331426	LEU	87.5695
3QZZ	142	LEU	6.534813	LEU	83.8050
3ZJS	142	LEU	6.289922	LEU	80.1179
1N45	147	LEU	6.115862	LEU	123.9670
2R7A	167	LEU	6.508147	LEU	132.6910
5O1L	171	LEU	5.743071	LEU	140.5170
2IIZ	255	LEU	6.075868	LEU	168.3090
2R7A	257	LEU	5.559331	LEU	156.1720
2IIZ	286	LEU	5.566800	LEU	170.9810
2IPS	417	LEU	6.792313	LEU	133.2130
2IPS	433	LEU	5.458537	LEU	130.0630
7C74	433	LEU	5.275537	LEU	124.6650
7DMR	433	LEU	5.225161	LEU	132.7140
2Q6N	437	LEU	5.864970	LEU	72.0648
3VP5	145	LYS	5.832567	LYS	85.9178
5O1M	167	LYS	5.125712	LYS	134.4970
1B2V	140	MET	6.218846	MET	173.7920
1DK0	140	MET	6.185917	MET	173.4760
1DKH	140	MET	6.519598	MET	172.2070
2CN4	140	MET	5.816277	MET	172.2930
4JET	147	MET	5.810508	MET	164.8890
4XZD	147	MET	6.297861	MET	157.8890
4Y1Q	147	MET	6.115760	MET	164.0570
4UZV	151	MET	5.908059	MET	159.1620
4CDP	241	MET	6.340896	MET	157.1200
2J0P	244	MET	6.821994	MET	155.7900
4MF9	257	MET	6.826627	MET	151.6460
5VEU	444	MET	6.285199	MET	65.6856
4I3Q	445	MET	5.975507	MET	65.1655
4NL5	23	PHE	5.580423	PHE	91.4353
2SPL	29	PHE	6.129536	PHE	109.5760
1B5M	35	PHE	5.848448	PHE	126.8820
1ICC	35	PHE	6.276818	PHE	121.2740
1U9U	35	PHE	6.094672	PHE	120.9680
2SPL	43	PHE	5.815167	PHE	96.0910

Table B.17: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
5CN5	43	PHE	5.981197	PHE	99.8337
4B8N	44	PHE	6.120000	PHE	119.7920
4JET	50	PHE	6.875792	PHE	101.1990
4Y1Q	50	PHE	6.555816	PHE	113.8000
4UZV	53	PHE	6.941930	PHE	134.2300
2CJ0	57	PHE	6.484645	PHE	126.1650
2CPO	57	PHE	6.473913	PHE	125.6230
2J18	57	PHE	6.534471	PHE	126.3090
1B5M	58	PHE	6.096500	PHE	85.0021
1ICC	58	PHE	6.182239	PHE	70.5320
4B8N	67	PHE	6.248829	PHE	78.7253
4UZV	67	PHE	5.984317	PHE	105.7360
1SY2	68	PHE	6.098374	PHE	105.5040
3MVF	68	PHE	6.146303	PHE	102.8610
3TGC	68	PHE	6.152796	PHE	103.4820
2VEB	74	PHE	6.405384	PHE	96.7886
3QZZ	74	PHE	6.218919	PHE	94.8642
3ZJS	74	PHE	6.270262	PHE	95.7239
3VP5	76	PHE	6.844578	PHE	108.6770
4JET	77	PHE	6.310922	PHE	57.4300
4XZD	77	PHE	6.275751	PHE	57.5972
4Y1Q	77	PHE	6.412846	PHE	49.1641
2VEB	93	PHE	5.810118	PHE	112.4610
3QZZ	93	PHE	6.033470	PHE	111.4380
3ZJS	93	PHE	5.922481	PHE	109.4020
2CJ0	103	PHE	6.182880	PHE	112.2600
2CPO	103	PHE	6.396792	PHE	112.7860
2J18	103	PHE	6.235843	PHE	111.5310
3VP5	112	PHE	6.509162	PHE	98.9329
4UZV	119	PHE	5.820671	PHE	139.8230
1SI8	132	PHE	6.553242	PHE	138.1490
1SI8	140	PHE	5.575451	PHE	139.2170
2VEB	145	PHE	6.211153	PHE	170.3740
3QZZ	145	PHE	6.192963	PHE	171.6250
3ZJS	145	PHE	6.059949	PHE	169.5920

Table B.17: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
1P3T	181	PHE	5.974488	PHE	104.9100
2CJ0	186	PHE	5.833496	PHE	170.8360
2CPO	186	PHE	5.891089	PHE	173.0070
2J18	186	PHE	5.882819	PHE	174.2510
2J0P	199	PHE	6.468406	PHE	116.5200
1IPH	206	PHE	6.665963	PHE	134.5530
1N45	207	PHE	5.975984	PHE	104.6170
1VGI	207	PHE	6.238995	PHE	106.2160
1IPH	214	PHE	5.767678	PHE	138.4550
2FC2	231	PHE	6.129726	PHE	115.0550
4CDP	243	PHE	5.994465	PHE	125.6670
2J0P	246	PHE	6.155004	PHE	127.9200
2IIZ	257	PHE	5.749045	PHE	119.3170
4MF9	259	PHE	5.680334	PHE	124.8600
7C74	347	PHE	6.478230	PHE	83.5884
7DMR	347	PHE	6.671472	PHE	87.2067
2BHJ	363	PHE	5.980185	PHE	116.4950
2Q6N	429	PHE	6.192258	PHE	80.7723
5VEU	434	PHE	6.084164	PHE	82.5712
4I3Q	435	PHE	6.161681	PHE	83.4925
1ZVI	584	PHE	6.009975	PHE	116.6380
2CJ0	28	PRO	6.127671	PRO	76.4322
2CPO	28	PRO	6.018197	PRO	69.8826
2J18	28	PRO	6.103023	PRO	75.1381
2CJ0	30	PRO	5.960531	PRO	65.8824
2CPO	30	PRO	6.017188	PRO	65.4937
2J18	30	PRO	5.936382	PRO	66.0535
1B5M	40	PRO	6.032548	PRO	84.9302
1ICC	40	PRO	6.016737	PRO	84.5709
1U9U	40	PRO	6.149502	PRO	87.3619
4B8N	49	PRO	6.182011	PRO	79.7519
1SI8	315	PRO	6.539721	PRO	121.9570
1IPH	393	PRO	6.703993	PRO	126.7810
2Q6N	428	PRO	6.945175	PRO	74.9040
5VEU	433	PRO	6.574196	PRO	65.9573

Table B.17: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
4I3Q	434	PRO	6.893037	PRO	69.3456
1B2V	42	SER	6.443386	SER	82.8367
1DK0	42	SER	6.540219	SER	80.4760
1DKH	42	SER	6.070312	SER	32.8371
2FC2	59	SER	6.581787	SER	146.0560
2E2Y	92	SER	6.454585	SER	115.2050
2SPL	92	SER	6.650791	SER	113.0460
5CN5	92	SER	6.529632	SER	111.5180
1P3T	117	SER	5.531584	SER	57.1608
1N45	142	SER	6.525024	SER	110.0660
1VGI	142	SER	5.700272	SER	125.4790
4MYP	205	SER	6.655356	SER	154.8290
6A2J	261	SER	6.949581	SER	84.4336
1QHU	266	SER	6.680148	SER	59.3970
1QJS	267	SER	6.730283	SER	71.5751
1IPH	414	SER	6.728176	SER	141.7910
1DK0	33	THR	6.991008	THR	13.7171
2R7A	52	THR	5.945515	THR	116.2990
2E2Y	67	THR	6.891096	THR	106.0790
3VP5	68	THR	6.164947	THR	105.7800
4XZD	82	THR	6.830323	THR	18.2203
1B2V	84	THR	6.798527	THR	18.8827
1DK0	84	THR	6.799510	THR	19.3165
1DKH	84	THR	6.267175	THR	31.3703
2CN4	84	THR	6.804573	THR	19.9645
1SY2	121	THR	6.333312	THR	142.1010
3MVF	121	THR	6.595150	THR	151.0630
3TGC	121	THR	6.343084	THR	149.1780
3VP5	130	THR	5.980868	THR	115.4180
1N45	135	THR	6.713859	THR	60.4070
1VGI	135	THR	6.883314	THR	58.3823
5O1M	168	THR	6.373467	THR	85.9567
6A2J	178	THR	6.772182	THR	86.8748
5O1L	194	THR	6.305648	THR	104.6020
5O1M	194	THR	6.409916	THR	101.5220

Table B.17: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
4MF9	208	THR	6.202558	THR	107.1870
5O1L	230	THR	6.574103	THR	168.0670
5O1M	230	THR	6.603918	THR	174.9180
2Q6N	302	THR	5.748396	THR	151.7240
4I3Q	309	THR	6.214341	THR	172.7070
5VEU	309	THR	5.895842	THR	174.8590
2E2Y	43	TRP	5.845537	TRP	95.5213
2FC2	56	TRP	5.737975	TRP	91.6643
3QZZ	60	TRP	6.491833	TRP	126.4880
3ZJS	60	TRP	6.366999	TRP	127.6490
4NL5	66	TRP	6.235302	TRP	112.7010
2R7A	68	TRP	6.192116	TRP	91.3335
1QHU	171	TRP	6.147194	TRP	135.3190
1QJS	171	TRP	6.211700	TRP	138.2760
2VEB	185	TRP	5.717992	TRP	165.6030
3QZZ	185	TRP	6.111800	TRP	156.0610
3ZJS	185	TRP	5.960798	TRP	163.3900
2BHJ	188	TRP	6.049049	TRP	95.4808
2CJ0	213	TRP	6.764355	TRP	116.4780
2J18	213	TRP	6.782850	TRP	117.0960
2FC2	234	TRP	6.837576	TRP	40.3488
1QHU	267	TRP	5.987630	TRP	70.5501
1QJS	268	TRP	6.230710	TRP	64.5387
2BHJ	366	TRP	6.764735	TRP	39.6654
1ZVI	409	TRP	5.660275	TRP	90.9270
1ZVI	587	TRP	6.843603	TRP	40.2585
1SY2	40	TYR	5.887937	TYR	145.2220
3MVF	40	TYR	6.759408	TYR	155.4560
3TGC	40	TYR	5.967215	TYR	142.7160
2O6P	52	TYR	6.682161	TYR	136.9010
2CN4	55	TYR	6.806239	TYR	136.9090
4JET	55	TYR	6.877273	TYR	128.1770
4XZD	55	TYR	6.821652	TYR	129.5380
4Y1Q	55	TYR	6.699820	TYR	130.2460
1SY2	58	TYR	6.964531	TYR	29.9485

Table B.17: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
1U9U	58	TYR	6.232812	TYR	75.1903
3ZJS	61	TYR	6.548411	TYR	78.2808
2R7A	67	TYR	4.159993	TYR	116.4820
1B2V	75	TYR	4.251885	TYR	132.4540
1DK0	75	TYR	4.346840	TYR	131.4420
1DKH	75	TYR	4.792830	TYR	125.4210
2CN4	75	TYR	4.345054	TYR	126.9230
4JET	75	TYR	4.420106	TYR	129.0130
4XZD	75	TYR	4.329954	TYR	127.5350
3VP5	91	TYR	6.574739	TYR	135.6840
2O6P	132	TYR	4.055037	TYR	132.9670
2O6P	136	TYR	5.148558	TYR	145.4090
3SIK	136	TYR	4.260470	TYR	131.7390
1B2V	137	TYR	6.232518	TYR	107.0750
1DK0	137	TYR	6.186950	TYR	107.9930
1DKH	137	TYR	6.409147	TYR	103.9420
2CN4	137	TYR	6.142879	TYR	102.8860
3SIK	140	TYR	5.120136	TYR	140.8870
1QHU	204	TYR	6.239544	TYR	82.8848
1QJS	204	TYR	6.225721	TYR	82.0806
4MYP	280	TYR	4.465249	TYR	129.7640
4MYP	289	TYR	5.900895	TYR	133.7170
1SI8	337	TYR	3.976560	TYR	101.8400
1IPH	415	TYR	4.218561	TYR	114.2710
1P3T	26	VAL	6.716946	VAL	118.5490
1SY2	36	VAL	6.479806	VAL	130.3660
3TGC	36	VAL	6.135653	VAL	128.7560
1B2V	37	VAL	5.425221	VAL	150.5390
1DK0	37	VAL	5.400636	VAL	154.2260
1DKH	37	VAL	5.642973	VAL	149.8520
1B5M	45	VAL	5.846522	VAL	132.2220
1ICC	45	VAL	5.992035	VAL	128.6010
1U9U	45	VAL	6.500194	VAL	133.1230
1SI8	53	VAL	6.238869	VAL	132.7600
4NL5	53	VAL	5.909472	VAL	175.0330

Table B.17: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
1B5M	61	VAL	6.074911	VAL	142.4900
1ICC	61	VAL	5.726742	VAL	157.5600
1U9U	61	VAL	6.163696	VAL	152.2510
2SPL	68	VAL	5.598014	VAL	111.2660
5CN5	68	VAL	5.556498	VAL	104.0070
4B8N	75	VAL	6.033658	VAL	149.8530
2VEB	89	VAL	5.917494	VAL	126.3020
3QZZ	89	VAL	5.927268	VAL	128.6650
3ZJS	89	VAL	5.790982	VAL	125.8290
2O6P	119	VAL	6.176593	VAL	171.6540
1SI8	125	VAL	6.016899	VAL	127.3950
1IPH	127	VAL	6.256166	VAL	129.5510
3VP5	131	VAL	5.568423	VAL	118.6510
3VP5	148	VAL	6.888565	VAL	110.6600
5O1L	152	VAL	6.293389	VAL	97.5310
5O1M	152	VAL	6.250877	VAL	96.3132
6A2J	175	VAL	6.202413	VAL	96.8786
6A2J	182	VAL	6.679490	VAL	146.8970
4CDP	192	VAL	5.600764	VAL	109.6320
2J0P	195	VAL	6.307524	VAL	111.4460
5O1L	197	VAL	6.648164	VAL	117.0650
5O1M	197	VAL	6.631076	VAL	113.6940
1IPH	199	VAL	6.294207	VAL	124.0950
2IIZ	228	VAL	5.315815	VAL	165.2710
2BHJ	346	VAL	6.643571	VAL	125.1020
2IPS	354	VAL	6.655642	VAL	133.4880
5VEU	369	VAL	6.886497	VAL	120.7080
1ZVI	416	VAL	5.960795	VAL	55.0798

Table B.18: HEC: All CA-CB-Fe Angles

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
5KPF	81	ALA	6.517051	ALA	45.2733
5LFT	81	ALA	6.400723	ALA	49.6961
5T8W	81	ALA	6.484127	ALA	46.8814
3EAH	147	ALA	6.240842	ALA	152.0380
2BC5	106	ARG	5.961420	ARG	119.2950
6WZA	106	ARG	6.631682	ARG	132.5260
1BBH	129	ARG	5.790808	ARG	148.1750
3EAH	149	ARG	5.803314	ARG	75.1674
3EAH	153	ARG	6.514542	ARG	70.9288
2BC5	99	ASN	6.936196	ASN	26.5703
3X15	12	CYS	6.451594	CYS	87.5164
5KPF	14	CYS	6.631432	CYS	91.6899
5LFT	14	CYS	6.598389	CYS	89.7859
5T8W	14	CYS	6.647516	CYS	89.3990
6XNK	14	CYS	6.275930	CYS	94.7801
2BH5	15	CYS	6.513509	CYS	93.4388
3X15	15	CYS	6.178945	CYS	124.5130
5KPF	17	CYS	6.098545	CYS	128.9880
5LFT	17	CYS	6.056595	CYS	131.2330
5T8W	17	CYS	6.188739	CYS	130.6870
6XNK	17	CYS	5.903640	CYS	129.1390
1W2L	18	CYS	6.554906	CYS	83.0319
2BH5	18	CYS	6.369197	CYS	129.9250
1W2L	21	CYS	6.223591	CYS	129.4480
2BC5	98	CYS	5.957326	CYS	83.1994
6WZA	98	CYS	5.774303	CYS	89.2313
2BC5	101	CYS	6.394766	CYS	122.7380
6WZA	101	CYS	6.455707	CYS	120.0850
1BBH	121	CYS	5.737156	CYS	88.6062
1BBH	124	CYS	6.272059	CYS	118.4660
3EAH	150	CYS	4.247423	CYS	109.9070
6VDQ	317	CYS	6.231170	CYS	153.4870
1S56	58	GLN	6.005777	GLN	114.9080
1BBH	17	GLU	6.940695	GLU	46.8470
3X15	16	HIS	4.360557	HIS	123.2520

Table B.18: HEC: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
5KPF	18	HIS	4.310334	HIS	121.8690
5LFT	18	HIS	4.342999	HIS	122.5120
5T8W	18	HIS	4.334295	HIS	122.3910
6XNK	18	HIS	4.599701	HIS	122.1970
2BH5	19	HIS	4.283790	HIS	122.4230
1W2L	22	HIS	4.350769	HIS	122.1140
1S56	81	HIS	4.475028	HIS	112.6780
2BC5	102	HIS	4.186908	HIS	96.2948
6WZA	102	HIS	4.440577	HIS	93.6577
1BBH	125	HIS	4.218890	HIS	95.2502
6VDQ	274	HIS	4.500421	HIS	121.1700
6VDQ	313	HIS	4.120545	HIS	123.2950
3X15	30	ILE	6.412845	ILE	143.9220
1W2L	61	ILE	6.839545	ILE	64.6202
6XNK	75	ILE	6.412701	ILE	119.2950
1S56	86	ILE	5.878780	ILE	163.7880
6VDQ	278	ILE	5.358791	ILE	112.0200
2BC5	3	LEU	6.742954	LEU	93.4646
6WZA	3	LEU	6.697674	LEU	97.4908
2BC5	10	LEU	6.154091	LEU	145.5220
6WZA	10	LEU	6.067786	LEU	145.9270
5KPF	32	LEU	6.145036	LEU	120.1710
5LFT	32	LEU	6.106815	LEU	122.2640
5T8W	32	LEU	5.994375	LEU	121.4370
6XNK	32	LEU	6.085909	LEU	119.5620
2BH5	39	LEU	5.728784	LEU	123.5750
1S56	54	LEU	5.947501	LEU	117.0640
5KPF	68	LEU	6.268124	LEU	84.1501
5LFT	68	LEU	6.315525	LEU	85.1852
5T8W	68	LEU	6.123569	LEU	85.5580
6VDQ	238	LEU	6.409586	LEU	130.4750
6VDQ	277	LEU	6.506868	LEU	130.8480
6XNK	79	LYS	3.938274	LYS	132.9060
2BH5	100	LYS	4.313747	LYS	174.4600
2BC5	7	MET	4.661903	MET	112.0730

Table B.18: HEC: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
6WZA	7	MET	4.611608	MET	112.1700
1BBH	19	MET	6.049470	MET	132.1620
1W2L	76	MET	4.403618	MET	95.5351
1S56	77	MET	6.187616	MET	79.9304
5KPF	80	MET	4.692154	MET	126.7040
5LFT	80	MET	4.757864	MET	124.0680
5T8W	80	MET	4.693021	MET	126.3770
1W2L	34	PHE	5.935685	PHE	94.2433
3X15	44	PHE	6.024333	PHE	118.7300
1S56	46	PHE	5.938368	PHE	100.7840
2BC5	65	PHE	6.201901	PHE	87.4034
6WZA	65	PHE	6.184290	PHE	90.1118
5KPF	82	PHE	6.311357	PHE	145.9170
5LFT	82	PHE	6.466458	PHE	143.5030
5T8W	82	PHE	6.527249	PHE	141.0090
2BH5	102	PHE	6.736126	PHE	125.9060
3EAH	319	PHE	6.137327	PHE	117.8130
6VDQ	320	PHE	6.121894	PHE	123.1650
3X15	25	PRO	6.252857	PRO	84.9462
5KPF	30	PRO	6.184028	PRO	77.6163
5LFT	30	PRO	6.179273	PRO	78.6390
5T8W	30	PRO	6.138272	PRO	79.9221
6XNK	30	PRO	5.900245	PRO	78.3181
1W2L	32	PRO	6.457693	PRO	80.5165
2BH5	37	PRO	6.202537	PRO	77.9642
5KPF	71	PRO	6.976183	PRO	151.2390
5LFT	71	PRO	6.983064	PRO	154.1260
5T8W	71	PRO	6.909375	PRO	148.7700
1W2L	77	PRO	6.071845	PRO	84.7339
2BH5	83	PRO	6.953188	PRO	141.6410
1W2L	60	SER	6.470812	SER	107.3410
6XNK	28	THR	6.983672	THR	95.9136
6VDQ	309	THR	6.443589	THR	99.5431
3EAH	144	TRP	5.647844	TRP	91.6868
6VDQ	271	TRP	5.880644	TRP	138.8540

Table B.18: HEC: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
3EAH	322	TRP	6.529256	TRP	42.5273
1BBH	16	TYR	4.795494	TYR	126.0380
1S56	33	TYR	6.252015	TYR	98.2768
1BBH	58	TYR	6.554347	TYR	118.4030
5KPF	67	TYR	5.922923	TYR	117.3570
5LFT	67	TYR	5.919346	TYR	117.9010
5T8W	67	TYR	5.858639	TYR	116.3210
6XNK	67	TYR	5.613420	TYR	126.9700
2BH5	79	TYR	5.535216	TYR	107.5970
1W2L	80	TYR	6.249808	TYR	159.9880
6VDQ	310	TYR	6.768220	TYR	57.7313
1W2L	75	VAL	6.753821	VAL	68.5700
1S56	80	VAL	6.205932	VAL	122.1110
2BH5	80	VAL	6.887770	VAL	86.0062
6XNK	83	VAL	6.004096	VAL	114.6820
1S56	94	VAL	6.626107	VAL	156.6730
1S56	126	VAL	6.029592	VAL	116.6120
3EAH	151	VAL	6.103944	VAL	58.7518

Table B.19: SRM: All CA-CB-Fe Angles

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
1ZJ8	468	ALA	6.774896	ALA	54.3434
3B0G	486	ALA	6.469408	ALA	52.3271
3VKP	486	ALA	6.471195	ALA	52.9419
3VLX	486	ALA	6.481752	ALA	51.8739
3VLY	486	ALA	6.503895	ALA	51.7331
3VLZ	486	ALA	6.507235	ALA	53.7924
5H8V	545	ALA	6.528336	ALA	49.2614
2AOP	83	ARG	5.905472	ARG	162.1930
1ZJ8	97	ARG	5.632921	ARG	148.8370

Table B.19: SRM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
2AKJ	109	ARG	5.624044	ARG	148.4620
3B0G	109	ARG	5.714505	ARG	157.7590
3VKP	109	ARG	5.727950	ARG	159.0060
3VLX	109	ARG	5.657293	ARG	157.8390
3VLY	109	ARG	5.670401	ARG	156.2520
3VLZ	109	ARG	5.666461	ARG	159.7330
5H8V	124	ARG	5.731236	ARG	158.1950
2AOP	153	ARG	6.898322	ARG	144.7120
1ZJ8	166	ARG	6.411696	ARG	157.1260
2AKJ	179	ARG	6.270969	ARG	150.8160
3B0G	179	ARG	6.332302	ARG	150.2730
3VKP	179	ARG	6.261289	ARG	149.5410
3VLX	179	ARG	6.332845	ARG	148.5140
3VLY	179	ARG	6.349458	ARG	149.9780
3VLZ	179	ARG	6.432708	ARG	147.1060
5H8V	193	ARG	6.748373	ARG	152.0550
2AOP	116	ASN	6.627004	ASN	95.1407
1ZJ8	465	ASN	6.589731	ASN	126.9150
2AOP	481	ASN	6.568014	ASN	121.7600
3B0G	483	ASN	6.105308	ASN	124.8060
3VKP	483	ASN	6.093849	ASN	125.9350
3VLX	483	ASN	6.149563	ASN	124.5220
3VLY	483	ASN	6.199685	ASN	124.0840
3VLZ	483	ASN	6.172324	ASN	122.9020
2AKJ	484	ASN	6.180565	ASN	125.4620
5H8V	542	ASN	6.517505	ASN	120.9920
1ZJ8	129	ASP	6.873987	ASP	96.5485
1ZJ8	467	CYS	4.642760	CYS	106.8380
2AOP	483	CYS	4.593058	CYS	115.6650
3B0G	485	CYS	4.334547	CYS	114.2180
3VKP	485	CYS	4.338921	CYS	113.1560
3VLX	485	CYS	4.333556	CYS	112.7580
3VLY	485	CYS	4.349260	CYS	114.5360
3VLZ	485	CYS	4.361247	CYS	115.6310
2AKJ	486	CYS	4.400598	CYS	106.3630

Table B.19: SRM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
5H8V	494	CYS	6.918908	CYS	129.0520
5H8V	544	CYS	4.294361	CYS	112.4810
2AOP	121	GLN	6.832109	GLN	146.9480
1ZJ8	134	GLN	6.870508	GLN	147.3840
5H8V	161	GLN	6.725078	GLN	141.5670
1ZJ8	207	LYS	5.279599	LYS	172.2200
1ZJ8	209	LYS	5.254105	LYS	132.2160
2AOP	215	LYS	5.521547	LYS	157.3800
2AOP	217	LYS	5.485034	LYS	135.7480
2AKJ	224	LYS	5.292960	LYS	179.3020
3B0G	224	LYS	5.579947	LYS	175.7930
3VKP	224	LYS	5.500133	LYS	175.8260
3VLX	224	LYS	5.605021	LYS	177.4260
3VLY	224	LYS	5.637976	LYS	177.5250
3VLZ	224	LYS	5.601385	LYS	175.4720
3VLY	226	LYS	5.485627	LYS	132.6280
3VLZ	226	LYS	5.641233	LYS	129.8350
5H8V	276	LYS	5.805329	LYS	174.1460
5H8V	278	LYS	5.495851	LYS	140.5820
1ZJ8	466	SER	6.539429	SER	46.1914
2AKJ	485	SER	6.504302	SER	45.1203
2AKJ	142	THR	6.814343	THR	112.5850
3B0G	142	THR	6.442796	THR	114.5110
3VKP	142	THR	6.428882	THR	114.3200
3VLX	142	THR	6.455248	THR	113.9840
3VLY	142	THR	6.452740	THR	113.0910
3VLZ	142	THR	6.394057	THR	112.9370
5H8V	156	THR	6.490994	THR	114.0040
3B0G	484	THR	6.402854	THR	31.8530
3VKP	484	THR	6.412766	THR	32.2678
3VLX	484	THR	6.401875	THR	31.6972
3VLY	484	THR	6.414362	THR	32.6034
3VLZ	484	THR	6.437540	THR	35.4494
1ZJ8	69	TYR	6.963349	TYR	168.2380
5H8V	106	TYR	6.992106	TYR	153.7720

Table B.20: VERDOHEME: All CA-CB-Fe Angles

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
2ZVU	28	ALA	6.962159	ALA	120.0970
3MOO	136	ASP	6.778611	ASP	23.6316
2ZVU	140	ASP	6.674210	ASP	26.6732
3MOO	24	GLU	6.275511	GLU	110.6430
2ZVU	29	GLU	6.221641	GLU	117.2590
3MOO	20	HIS	4.614778	HIS	111.0890
2ZVU	25	HIS	4.603252	HIS	110.7510
3MOO	134	LEU	6.100073	LEU	77.1733
2ZVU	138	LEU	6.249768	LEU	76.7687
3MOO	201	PHE	5.958999	PHE	104.2170
2ZVU	207	PHE	6.037412	PHE	105.4400
3MOO	138	SER	5.886820	SER	125.3120
2ZVU	142	SER	6.048311	SER	126.2110
2ZVU	135	THR	6.765195	THR	58.6713
3MOO	131	VAL	6.796515	VAL	60.1702
1TWN	140	ASP	6.273979	ASP	27.4847
1TWR	140	ASP	6.553790	ASP	27.4184
1TWN	29	GLU	6.123574	GLU	100.1730
1TWR	29	GLU	6.517157	GLU	103.1100
1TWN	25	HIS	4.673370	HIS	113.5160
1TWR	25	HIS	4.786588	HIS	108.8640
1TWN	138	LEU	6.399559	LEU	75.1317
1TWR	138	LEU	6.579770	LEU	75.0669
1TWN	207	PHE	6.263716	PHE	105.9700
1TWR	207	PHE	6.447849	PHE	107.0750
1TWN	142	SER	6.035867	SER	114.7150
1TWR	142	SER	6.195017	SER	129.2760
1TWN	135	THR	6.865192	THR	60.8151

B.6 CA-CB-Fe Angles of Closest Residues

Table B.21: HEM: CA-CB-Fe Angles of Closest Residues

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
1B2V	75	TYR	4.251885	TYR	132.4540
1B2V	32	HIS	4.667618	HIS	116.3150
1B2V	83	HIS	5.366599	HIS	102.9160
1B5M	63	HIS	4.211990	HIS	125.8380
1B5M	39	HIS	4.456809	HIS	101.8130
1DK0	75	TYR	4.346840	TYR	131.4420
1DK0	32	HIS	4.556145	HIS	116.4470
1DK0	83	HIS	5.314133	HIS	102.7520
1DKH	75	TYR	4.792830	TYR	125.4210
1DKH	32	HIS	5.099382	HIS	121.3750
1DKH	83	HIS	5.223800	HIS	122.9600
1ICC	63	HIS	4.451283	HIS	114.1290
1ICC	39	HIS	4.542187	HIS	101.5070
1IPH	415	TYR	4.218561	TYR	114.2710
1IPH	411	ARG	5.321024	ARG	108.2630
1IPH	128	HIS	5.713777	HIS	129.2180
1N45	25	HIS	4.545004	HIS	112.7600
1P3T	23	HIS	4.573926	HIS	111.7580
1P3T	117	SER	5.531584	SER	57.1608
1QHU	265	HIS	4.200094	HIS	121.1810
1QHU	213	HIS	4.734866	HIS	114.5350
1QHU	267	TRP	5.987630	TRP	70.5501
1QJS	266	HIS	4.484379	HIS	120.9930
1QJS	213	HIS	4.696712	HIS	122.0930
1QJS	171	TRP	6.211700	TRP	138.2760
1SI8	337	TYR	3.976560	TYR	101.8400
1SI8	333	ARG	5.247624	ARG	116.1170
1SI8	140	PHE	5.575451	PHE	139.2170
1SY2	59	HIS	4.045387	HIS	126.3700
1SY2	40	TYR	5.887937	TYR	145.2220
1SY2	123	LEU	5.902915	LEU	147.6300
1U9U	63	HIS	4.417873	HIS	116.0130
1U9U	39	HIS	4.589294	HIS	102.2750
1VGI	25	HIS	4.646180	HIS	113.1630
1ZVI	415	CYS	4.181834	CYS	112.7440

Table B.21: HEM: CA-CB-Fe Angles of Closest Residues *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
1ZVI	409	TRP	5.660275	TRP	90.9270
2BHJ	194	CYS	4.487497	CYS	118.0500
2BHJ	193	ARG	5.745098	ARG	61.6429
2CJ0	29	CYS	4.390905	CYS	117.5660
2CJ0	31	ALA	5.440871	ALA	114.8710
2CJ0	183	GLU	5.716050	GLU	106.0810
2CN4	75	TYR	4.345054	TYR	126.9230
2CN4	83	HIS	5.251875	HIS	107.5140
2CN4	140	MET	5.816277	MET	172.2930
2CPO	29	CYS	4.443549	CYS	118.1890
2CPO	31	ALA	5.505123	ALA	115.0400
2CPO	183	GLU	5.799506	GLU	105.9460
2E2Y	93	HIS	4.514535	HIS	114.4980
2E2Y	68	ILE	5.517060	ILE	97.7283
2E2Y	43	TRP	5.845537	TRP	95.5213
2FC2	62	CYS	4.482879	CYS	112.5820
2FC2	56	TRP	5.737975	TRP	91.6643
2IIZ	224	HIS	4.533607	HIS	124.3380
2IIZ	242	ARG	5.236889	ARG	162.0190
2IIZ	228	VAL	5.315815	VAL	165.2710
2IPS	351	HIS	4.125792	HIS	94.9759
2IPS	433	LEU	5.458537	LEU	130.0630
2IPS	108	ASP	5.870986	ASP	152.6010
2J0P	196	HIS	4.310325	HIS	111.1620
2J0P	102	ARG	5.002395	ARG	139.6090
2J0P	246	PHE	6.155004	PHE	127.9200
2J18	29	CYS	4.359887	CYS	118.4250
2J18	31	ALA	5.457126	ALA	114.2550
2J18	183	GLU	5.722472	GLU	107.1960
2O6P	132	TYR	4.055037	TYR	132.9670
2O6P	136	TYR	5.148558	TYR	145.4090
2O6P	48	ILE	5.365972	ILE	141.3220
2Q6N	436	CYS	4.305637	CYS	109.8240
2Q6N	298	ALA	5.672036	ALA	129.8410
2R7A	67	TYR	4.159993	TYR	116.4820

Table B.21: HEM: CA-CB-Fe Angles of Closest Residues *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
2R7A	169	ALA	5.223004	ALA	132.6020
2R7A	257	LEU	5.559331	LEU	156.1720
2SPL	93	HIS	4.578545	HIS	112.4730
2SPL	68	VAL	5.598014	VAL	111.2660
2SPL	43	PHE	5.815167	PHE	96.0910
2VEB	120	HIS	4.471709	HIS	110.4880
2VEB	185	TRP	5.717992	TRP	165.6030
2VEB	93	PHE	5.810118	PHE	112.4610
3MVF	59	HIS	4.066882	HIS	126.0770
3MVF	42	ALA	5.827660	ALA	147.3790
3MVF	123	LEU	5.891492	LEU	147.9850
3QZZ	120	HIS	4.599066	HIS	109.3460
3QZZ	89	VAL	5.927268	VAL	128.6650
3QZZ	93	PHE	6.033470	PHE	111.4380
3SIK	136	TYR	4.260470	TYR	131.7390
3SIK	140	TYR	5.120136	TYR	140.8870
3SIK	54	ARG	6.090293	ARG	163.0460
3TGC	59	HIS	4.100823	HIS	124.3700
3TGC	123	LEU	5.908675	LEU	148.3100
3TGC	40	TYR	5.967215	TYR	142.7160
3VP5	149	HIS	4.350835	HIS	100.8200
3VP5	72	HIS	4.371971	HIS	101.6570
3VP5	131	VAL	5.568423	VAL	118.6510
3ZJS	120	HIS	4.427156	HIS	110.7000
3ZJS	89	VAL	5.790982	VAL	125.8290
3ZJS	93	PHE	5.922481	PHE	109.4020
4B8N	71	HIS	4.416116	HIS	119.3920
4B8N	48	HIS	4.479396	HIS	104.9040
4CDP	193	HIS	4.417630	HIS	109.7720
4CDP	100	ARG	5.360373	ARG	139.0430
4CDP	192	VAL	5.600764	VAL	109.6320
4I3Q	442	CYS	4.085782	CYS	103.9950
4I3Q	305	ALA	5.305272	ALA	115.6050
4JET	75	TYR	4.420106	TYR	129.0130
4JET	81	HIS	5.381133	HIS	121.2740

Table B.21: HEM: CA-CB-Fe Angles of Closest Residues *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
4JET	40	ARG	5.660400	ARG	117.6700
4MF9	209	HIS	4.606487	HIS	108.6490
4MF9	112	ARG	5.056393	ARG	134.9890
4MF9	259	PHE	5.680334	PHE	124.8600
4MYP	280	TYR	4.465249	TYR	129.7640
4MYP	289	TYR	5.900895	TYR	133.7170
4MYP	293	ALA	6.207799	ALA	133.2580
4NL5	75	HIS	4.473936	HIS	117.7090
4NL5	7	ASN	5.402231	ASN	170.5520
4NL5	23	PHE	5.580423	PHE	91.4353
4UZV	106	HIS	4.502311	HIS	110.2430
4UZV	119	PHE	5.820671	PHE	139.8230
4UZV	111	ILE	5.897899	ILE	140.3930
4XZD	75	TYR	4.329954	TYR	127.5350
4XZD	81	HIS	5.263108	HIS	114.4420
4XZD	40	ARG	5.892195	ARG	118.8830
4Y1Q	81	HIS	5.294289	HIS	126.8310
4Y1Q	40	ARG	5.725205	ARG	121.1480
4Y1Q	147	MET	6.115760	MET	164.0570
5CN5	93	HIS	4.575365	HIS	113.1870
5CN5	68	VAL	5.556498	VAL	104.0070
5CN5	64	HIS	5.804727	HIS	107.1420
5O1L	198	HIS	4.305405	HIS	102.4410
5O1L	171	LEU	5.743071	LEU	140.5170
5O1L	222	ILE	6.024951	ILE	133.4090
5O1M	198	HIS	4.392715	HIS	100.3070
5O1M	167	LYS	5.125712	LYS	134.4970
5O1M	222	ILE	6.241067	ILE	136.2240
5VEU	441	CYS	4.349464	CYS	106.7690
5VEU	309	THR	5.895842	THR	174.8590
6A2J	216	HIS	4.601722	HIS	122.2890
6A2J	278	HIS	4.655598	HIS	124.6210
7C74	351	HIS	4.494179	HIS	92.7950
7C74	433	LEU	5.275537	LEU	124.6650
7C74	105	GLN	5.667218	GLN	97.8161

Table B.21: HEM: CA-CB-Fe Angles of Closest Residues *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
7DMR	351	HIS	4.201640	HIS	96.7615
7DMR	433	LEU	5.225161	LEU	132.7140
7DMR	105	GLN	5.517249	GLN	100.6130

Table B.22: HEC: CA-CB-Fe Angles of Closest Residues

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
1BBH	125	HIS	4.218890	HIS	95.2502
1BBH	16	TYR	4.795494	TYR	126.0380
1BBH	121	CYS	5.737156	CYS	88.6062
1S56	81	HIS	4.475028	HIS	112.6780
1S56	86	ILE	5.878780	ILE	163.7880
1S56	46	PHE	5.938368	PHE	100.7840
1W2L	22	HIS	4.350769	HIS	122.1140
1W2L	76	MET	4.403618	MET	95.5351
1W2L	34	PHE	5.935685	PHE	94.2433
2BC5	102	HIS	4.186908	HIS	96.2948
2BC5	7	MET	4.661903	MET	112.0730
2BC5	98	CYS	5.957326	CYS	83.1994
2BH5	19	HIS	4.283790	HIS	122.4230
2BH5	100	LYS	4.313747	LYS	174.4600
2BH5	79	TYR	5.535216	TYR	107.5970
3EAH	150	CYS	4.247423	CYS	109.9070
3EAH	144	TRP	5.647844	TRP	91.6868
3X15	16	HIS	4.360557	HIS	123.2520
3X15	44	PHE	6.024333	PHE	118.7300
3X15	15	CYS	6.178945	CYS	124.5130
5KPF	18	HIS	4.310334	HIS	121.8690
5KPF	80	MET	4.692154	MET	126.7040
5KPF	67	TYR	5.922923	TYR	117.3570
5LFT	18	HIS	4.342999	HIS	122.5120

Table B.22: HEC: CA-CB-Fe Angles of Closest Residues *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
5LFT	80	MET	4.757864	MET	124.0680
5LFT	67	TYR	5.919346	TYR	117.9010
5T8W	18	HIS	4.334295	HIS	122.3910
5T8W	80	MET	4.693021	MET	126.3770
5T8W	67	TYR	5.858639	TYR	116.3210
6VDQ	313	HIS	4.120545	HIS	123.2950
6VDQ	274	HIS	4.500421	HIS	121.1700
6VDQ	278	ILE	5.358791	ILE	112.0200
6WZA	102	HIS	4.440577	HIS	93.6577
6WZA	7	MET	4.611608	MET	112.1700
6WZA	98	CYS	5.774303	CYS	89.2313
6XNK	79	LYS	3.938274	LYS	132.9060
6XNK	18	HIS	4.599701	HIS	122.1970
6XNK	67	TYR	5.613420	TYR	126.9700

Table B.23: SRM: CA-CB-Fe Angles of Closest Residues

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
1ZJ8	467	CYS	4.642760	CYS	106.838
1ZJ8	209	LYS	5.254105	LYS	132.216
1ZJ8	207	LYS	5.279599	LYS	172.220
2AKJ	486	CYS	4.400598	CYS	106.363
2AKJ	224	LYS	5.292960	LYS	179.302
2AKJ	109	ARG	5.624044	ARG	148.462
2AOP	483	CYS	4.593058	CYS	115.665
2AOP	217	LYS	5.485034	LYS	135.748
2AOP	215	LYS	5.521547	LYS	157.380
3B0G	485	CYS	4.334547	CYS	114.218
3B0G	224	LYS	5.579947	LYS	175.793
3B0G	109	ARG	5.714505	ARG	157.759
3VKP	485	CYS	4.338921	CYS	113.156

Table B.23: SRM: CA-CB-Fe Angles of Closest Residues *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
3VKP	224	LYS	5.500133	LYS	175.826
3VKP	109	ARG	5.727950	ARG	159.006
3VLX	485	CYS	4.333556	CYS	112.758
3VLX	224	LYS	5.605021	LYS	177.426
3VLX	109	ARG	5.657293	ARG	157.839
3VLY	485	CYS	4.349260	CYS	114.536
3VLY	226	LYS	5.485627	LYS	132.628
3VLY	224	LYS	5.637976	LYS	177.525
3VLZ	485	CYS	4.361247	CYS	115.631
3VLZ	224	LYS	5.601385	LYS	175.472
3VLZ	226	LYS	5.641233	LYS	129.835
5H8V	544	CYS	4.294361	CYS	112.481
5H8V	278	LYS	5.495851	LYS	140.582
5H8V	124	ARG	5.731236	ARG	158.195

Table B.24: VERDOHEME: CA-CB-Fe Angles of Closest Residues

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
2ZVU	25	HIS	4.603252	HIS	110.751
3MOO	20	HIS	4.614778	HIS	111.089
1TWN	25	HIS	4.673370	HIS	113.516
1TWR	25	HIS	4.786588	HIS	108.864

This is an attempt at referencing the tables above.

figure reference **??** table reference **??**

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.