Structural Analysis of Hemoprotein Binding Sites

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Acknowledgements

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

Thanks to everyone who taught me something during this program.

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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

Hemoproteins are able to catalyze an extraordinarily broad range of reactions. This class of proteins includes cytochrome P450s and peroxidases, among many others. Hemoproteins by definition include heme to achieve their chemistry; but heme molecules themselves vary considerably, and different heme molecules are employed depending on the function of a particular hemoprotein. At present, there is a knowledge gap in the literature of the structural features required to bind heme in hemoprotein binding sites.

In this study, we investigated the binding environments of heme-b, heme-c, siroheme, and verdoheme. A high-throughput framework was developed to generate, process, and analyze data derived from the Protein Data Bank (PDB) files used in the study. Amino acid frequencies, volume, surface areas, and angular relations within the heme binding sites were all obtained and examined for a diverse set of hemoproteins. Overall, we find that nonpolar residues and their interactions with heme may be of greater importance to heme binding than previously thought, suggesting that polar interactions, while necessary, are insufficient to efficiently bind heme. We also report several values for binding pocket volumes, surface areas, and angular data that may be of utility in artificial metalloenzyme design. The framework developed for this study is highly adaptable and may facilitate similar investigations for other proteins and ligands.

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Lay Summary

We investigated how heme, a molecule involved in many biological processes, binds to proteins. The study was conducted computationally. 3D structures of proteins were downloaded from a database, and run through software specialized for viewing molecules. This software was used to examine the region on the protein where heme binds (binding pocket). The software also predicted the volume and surface areas of the binding pocket. The data produced were analyzed using statistical software.

We found that a greater proportion of the binding pocket associates with the hydrophobic and uncharged parts of the heme molecules more frequently, and therefore likely more strongly, than previously thought. These results suggest that these hydrophobic, electrically inert parts of the pockets may be very important to consider when studying, or designing proteins containing heme. We also report the volume and surface area data that were predicted, which support the above conclusion and may also be of help when studying or designing these proteins.

Introduction

Proteins that contain metal ion cofactor(s) are known as metalloproteins, and they compose approximately 40% of all proteins. The metal ion can be free, or complexed with another molecule. One such molecule is heme, a complex of iron and a porphyrin ring. Heme is employed by many metalloproteins to catalyze a broad range of reactions[1].

There are many types of heme; but all of them are a coordination complex composed of an iron atom coordinated and bound to a modified porphyrin ring. Porphyins are composed of four pyrrole subunits (pentagonal structures of four carbons and a nitrogen) that are bound together via methine (i.e. carbon) bridges. Porphyrins are considered macrocycles, molecules with large ring structures. The ring within porphyrins is heterocyclic, and considered aromatic, and therefore acts as a large resonant structure capable of transferring electrons. Coupled with an iron atom to enable reduction-oxidation reactions and the macrocycle of the porphyrin ring, the overall heme complex is therefore highly suited for reactions involving electron transfer[2].

Proteins containing heme are known as hemoproteins - hemoglobin and myoglobin are well-known examples, using heme to store and transport oxygen. Other examples of hemoproteins are peroxidases, catalases (a type of peroxidase), nitric oxide synthases, heme oxygenases, and cytochrome p450s. Peroxidases and catalases catalyze oxidation-reduction reactions using a histidine-bound heme, with catalases in particular specializing in the decomposition of hydrogen peroxide. Nitric oxide synthases catalyze the reaction of L-arginine into nitric oxide, which is vitally important to cellular signaling [1]. Free heme molecules may be released upon degradation of hemoproteins (especially hemoglobin), however, heme is prooxidative

and therefore toxic to cells and must be cleared. Heme oxygenases assist in the degradation of heme, and are regarded as potential therapeutics, due to anti-inflammatory effects[3].

The enzymes with arguably the most potential applications, cytochrome P450s function as powerful monooxygenases. They participate in many reactions: capable oxidizing a wide range of substrates, including carbohydrates, steroids, fatty acids; catalyzing hormone degradation and synthesis; and degrading the majority of drugs[1]. Due to their extraordinary utility and range of reactions, cytochrome p450s are of great interest in the protein engineering field. Cytochrome P450s have the potential to be used in industrial biocatalysis, e.g. in pharmaceutical production, bioremediation of environmental pollutants[4, 5]. The limiting factor preventing its deployment has been the struggle to increase enzymatic efficiency and therefore yield of processes employing the enzyme[6, 7].

Thus far, only heme-b and its respective hemoproteins have been discussed (although heme-b is the most abundant and most employed type of heme). Other types of heme are structurally and chemically different, and are used to achieve different chemical reactions. In this study, we examined heme-b, heme-c, verdoheme, and siroheme. Their structures are shown in Figures 1-5, and each heme is individually discussed below.

0.1 Types of Heme

0.1.1 Heme-b

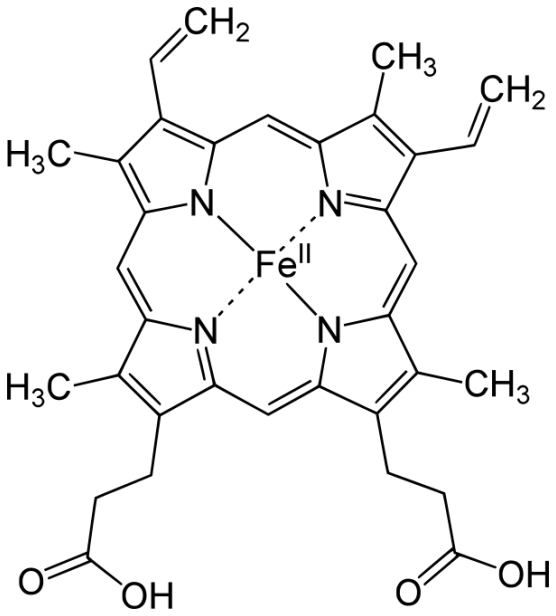

Figure 1: Heme-b (HEM)

The most common heme is heme-b. It is employed by the vast majority of hemoproteins. It is composed of an iron and porphyrin ring complex with attached vinyl and ethyl groups, and with the addition of two propionate groups. The iron atom is usually coordinated to a histidine or cysteine, depending on the enzyme[1, 2].

The two propionate groups stabilize the heme in the pocket by forming polar interactions with salt bridges formed by arginine residues in the binding environment[8]. This behavior is the same for heme-b and likely verdoheme. It has also been suggested that the propionate groups may also serve to exclude solvent from the binding environment, potentially acting to expel and repel water molecules [9].

0.1.2 Heme-c

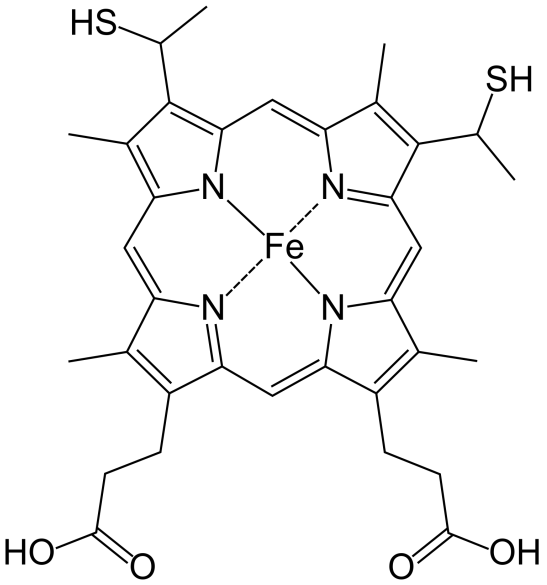

Figure 2: Heme-c (HEC)

Heme-c is derived from heme-b. It is fairly similar to heme, with two notable differences: the iron atom binds, with few exceptions, covalently to cysteine residues in the binding pocket; and its two vinyl groups form thioether bonds with amino acids in the protein binding pocket. Its function is much more specific than heme-b, mostly serving as an electron carrier rather than catalyzing a plethora of reactions. The reason for this is not abundantly clear, but several studies suggest that because of its covalent bonding, heme-c has an electronic potential that is can be far lower and in general more broad, and more specifiable, than heme-b. [2, 10]

0.1.3 Siroheme

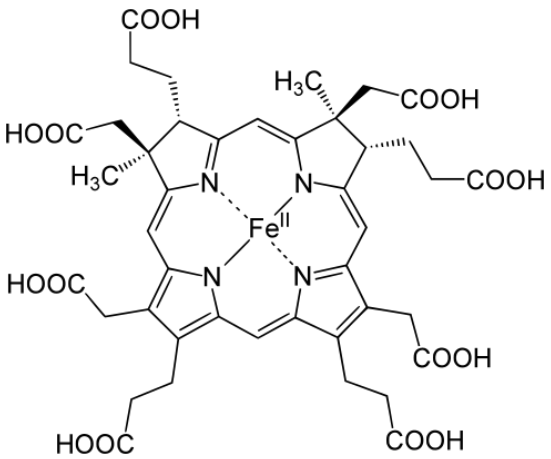

Figure 3: Siroheme (SRM)

Siroheme is even more limited in its applications, but highly specialized for its role. It is still an iron atom-porphyrin coordination complex, but it contains far more carboxyl and propionate groups than the other types of heme, making it highly polar. It is used exclusively in sulfite and nitrite reductases, which catalyze the reduction of the sulfates and nitrates plants uptake from the ground, providing the sources of nitrogen and sulfur used to produce nitrogen and sulfur-containing amino acids[11]. The reason for the use of siroheme in this reaction rather than heme-b is not completely understood. But one study suggests that the bridge that siroheme forms between its catalyic iron atom, and the protein matrix environment (which also necessarily involves another cofactor, a cluster of cubane for electron transfer and provision) is more efficient at channeling electrons than the bridge that could be formed by heme.[12]

0.1.4 Verdoheme

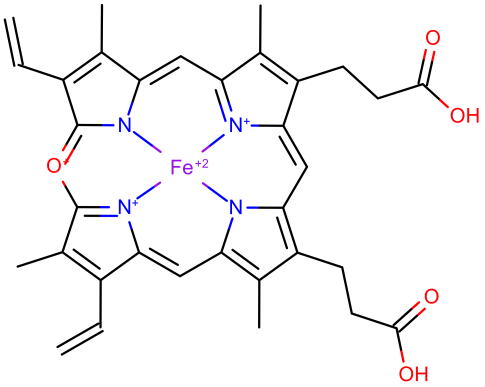

Figure 4: Verdoheme (VEA)

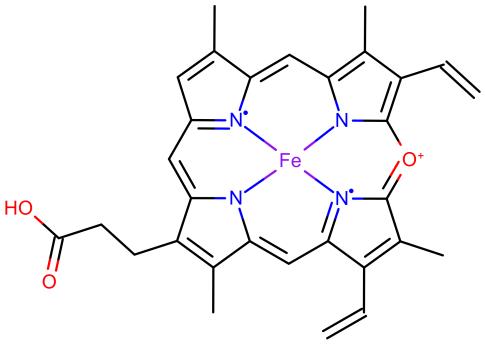

Figure 5: Verdoheme (VER)

Lastly, verdoheme is an intermediate product in the degradation of heme-b by heme oxygenase. When heme oxygenase degrades heme-b, biliverdin, carbon monoxide, and iron are produced; verdoheme is the precusor to bilverdin[13, 14]. While a product of prior reactions wthin heme oxygenase, verdoheme appears to be oriented and bound differently [15]. The two structures used in the study, VEA and

VER, are verdoheme at different stages of degradation, either partially oxidized or containing one less propionate group.

In summary, heme molecules can have very different structures and functions; they enable and catalyze an extraordinary amount, and extraordinarily diverse set of chemical reactions. They are important, not only as a study of how one class of molecule can be involved in a broad swath of reactions, but because hemoproteins have the potential to be of great value in biocatalysis, bioremediation, and pharmaceutical applications.

There is a significant barrier to the employment of hemoproteins in these areas, however: improving their efficiency far beyond what is found in nature. This is the field of artifical metalloproteins, or metalloenzymes: engineering metalloenzymes to improve them; increasing efficiency, stability, or even to introduce new reactions to heme's repetoire.

There are multiple methods employed to design these molecules, but rational design in particular (basically, the mutation of certain residues based on an understanding of the structure-function relationships) is at least partially hampered by an incomplete understanding of the binding environment for heme. For example, the importance of the binding environment was noted in a study seeking to design *de novo* heme-c based enzymes, and found the binding environment likely to be of importance in modulating redox potential [16].

A fairly recent study conducted a structural analysis of 125 hemoprotein chains[17]. The study suggested hemoproteins undergo small conformational changes during binding; and that apo-form (ligand-containing) proteins may therefore be suitable for bioinformatics-based prediction and protein design. Additionally, the heme binding environments for both heme-b and heme-c were analyzed, and relative frequencies per amino acid were reported. Cysteine, histidine, phenylalanine, methionine, and tyrosine were found to be the most abundant residues within the binding environments of both heme-b and heme-c.

The aforementioned study was published in 2011 – since then the PDB has been populated with far more hemoproteins. The focus of the study was on conformational

differences induced by heme-binding, rather than the binding environment, although the relative frequencies of amino acids were reported. Interactions of the more abundant residues with heme-b or heme-c, including interactions with the porphyrin ring, were briefly discussed and this discussion will not be reproduced here.

In this study, we present research focused on elucidating the binding environment of multiple heme molecules: heme-b (HEM), heme-c (HEC), siroheme (SER), and verdoheme (VEA/VER). A diverse set of PDBs was assembled. UCSF Chimera was used to both extract and predict properties of a diverse set of hemoproteins. R was used to analyze the results. A robust and high-throughput framework was constructed to process the datasets for each heme molecule, requiring only inputs of which ligand was to be examined per dataset.

The properties extracted and predicted of the heme molecules' binding environments were: the amino acid frequencies; the distances of the amino acids from the heme iron; the volume of the binding pocket; and the surface areas of both the hemes and the binding pocket. These data can be expected to be of use, or at least of interest, to efforts in artifical metalloenzyme design.

Additionally, angular data for the residues within the binding environment were obtained. These data were produced more for exploratory purposes and are not discussed extensively in this study. Specifically, planar angles and the angle between residues' alpha-carbon, beta-carbon, and heme iron (CA-CB-Fe) were obtained.

These results may be of use in rational design of hemoproteins in future studies, or at least, improve the understanding of the heme binding environment.

1 Methods

All scripts (as well as raw data, results, and this document) are available on GitHub[18].

1.1 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 superimposed 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=13), SRM (n=9), VER (n=2) and VEA (n=2), which are merged 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.

1.2 Pre-processing

Many of the PDBs downloaded were multimeric structures. The number of subunits per protein would skew results and overrepresent especially large multimeric proteins. Therefore, to only allow for one heme binding site per PDB, 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. Part of the script is reproduced below:

```
from chimera import runCommand as rc
# select chain A, a single unit
rc("sel :.a")
# select everything else
rc("sel invert sel")
# delete everything else besides that chain A
rc("del sel")
# now save the monomer:
rc(("write format pdb 0 "+unexpandedResultPath+activeLigand+"/%s")%
  (fn + ".mono.pdb"))
```

1.3 Processing Monomers

UCSF-Chimera was used to generate all data in this study. Multiple Python 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 potentially 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 cutoffs are selected arbitrarily, data from the 5A and 7A runs are overlaid in the figures reported in Appendix A. Data tables are also provided in Appendix B.

1.3.1 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.

1.3.2 Volume Calculations

Volume of the binding pocket was predicted via Surfnet [19], and 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). Surfnet is the molecular volume calculation tool implemented within UCSF Chimera. The script used selects the residues around heme to consider as the bounds of the pocket, but effectively ignores heme's presence as its calculates the volume, as if the pocket were empty:

```
from chimera import runCommand as rc
# Select the atoms within 7A of heme.
#Then, of that selection, keep everything but heme.
rc("sel :"+activeLigand+" za < "+angstromDistance)
# this is the syntax that accomplishes our desired selection
rc("sel sel &~:"+activeLigand)
interface_surfnet("sel","sel")
rc("sop split #") # acquire the individual pockets that have been generated
```

```
rc("measure volume #") # measures volume of individual pockets
# in R we keep only the largest volume
```

Surfnet, at least in this investigation, was prone to generating very small volumes. During analysis these were removed and only the largest volume generated is recorded, since the largest volume generated and identified is most likely the binding pocket. Two figures below demonstrate a run where one good pocket is produced, and one where a few very small "bubbles" are generated:

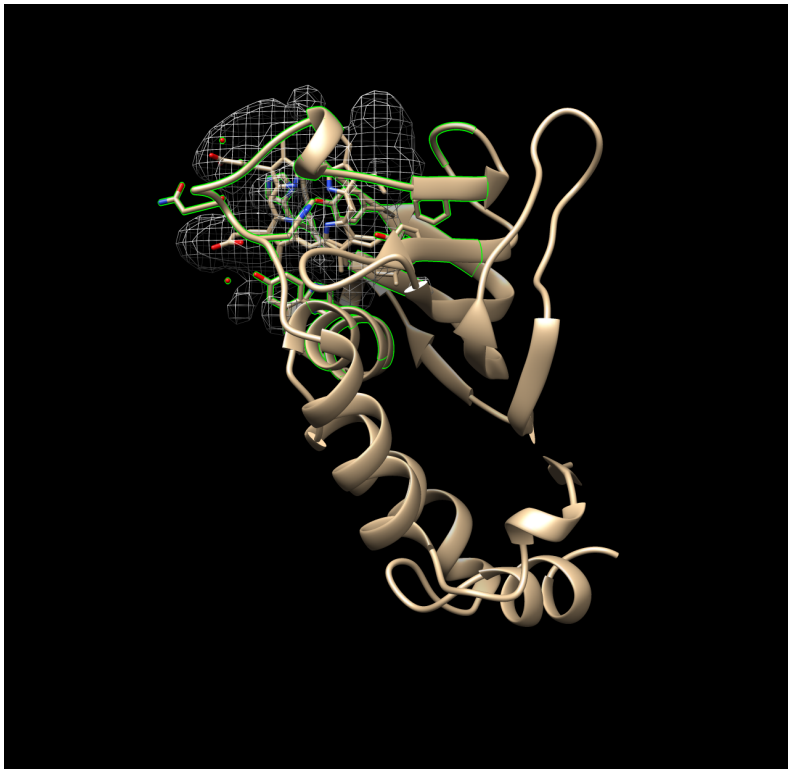

Figure 1.1: Good Example of Surfnet Run (1B2V)

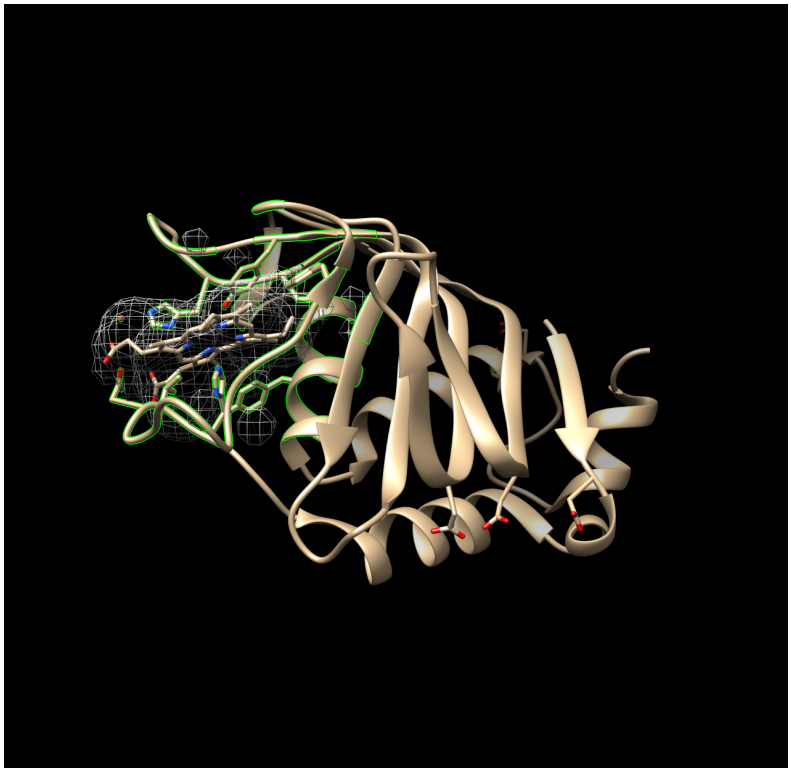

Figure 1.2: Non-Ideal Example of Surfnet Run (1DKH)

1.3.3 Surface Area Calculations

Solvent excluded and solvent accessible surface areas of both the ligand and the binding pocket were calculated using Chimera's "surf" algorithm, which itself is an implementation of a program called MSMS [20].

These two measures are similar but not the same. Solvent accessible surface area represents the surface area of the protein that a solvent molecule (i.e. water) may interact with. It is calculated by rolling a sphere on the Van der Waals surface of the protein, and the *center of the sphere* is recorded as the bounds of the accessible surface area. Solvent excluded surface area is calculated the same way, rolling a sphere on the Van der Waals surface of the protein, but instead the *point of contact of the sphere against the Van der Waals surface* is recorded as the excluded surface area. The solvent excluded surface area may therefore be considered the bounds of the protein itself, versus the solvent accessible surface area, which can be considered the bounds at which a solvent may interact with the protein[20].

1.3.4 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. This was achieved using a built-in function of chimera; the syntax is not straightforward, but part of the script is shown below. 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.

```
from chimera import runCommand as rc
#select and define the Fe atom
rc("sel :HEM@Fe")
# index to acquire the one atom selected
fe = chimera.selection.currentAtoms()[0]
# select all atoms within angstromDistance of Fe (also de-selects Fe)
rc("sel sel za < "+settings.angstromDistance)
# define this selection of atoms within distance as a list
nearbyAtoms = chimera.selection.currentAtoms()
# parse and print the distances (and coordinates) of these atoms
for i in nearbyAtoms:
  print "Atom being analyzed...", i, "... Distance to Fe...",
  #prints distance between atom i and the Fe atom
  i.coord().distance(fe.coord())
```

The data produced in this step therefore include the mean distance of each amino acid. Distances are traceable per residue and atoms in each residue; this data was used to construct the distributions of amino acids over distance, and the angular data below are cross-referenced with this list of distances.

1.3.5 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. This employed the "define axis", and "angle" functions of Chimera; the Axes/Planes/Centroids Structural Analysis function of Chimera via GUI.

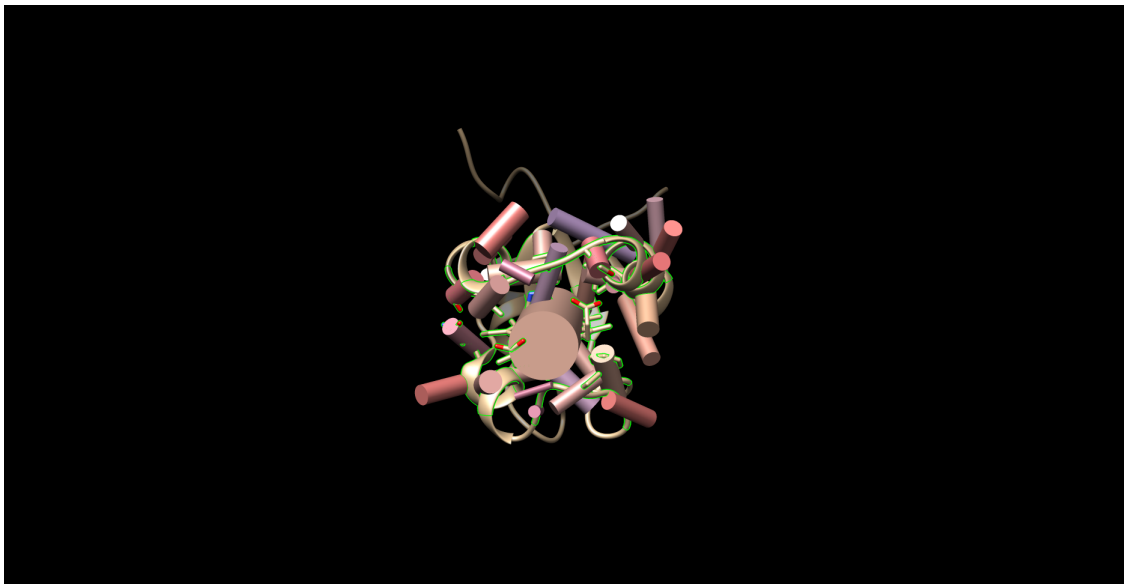

Figure 1.3: Example of Planar Angles Calculation (1B5M)

1.3.6 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.

1.4 Import to R

The data produced by Chimera and the Python scripts were stored as .txt files. These files were imported to R and processed from .txt files into organized data formats. All plots and tables were constructed using R and imported directly to this document using Rmarkdown.

2

Results and Discussion

2.1 Analysis of Residues Nearby Each Heme Molecule

We began the study by acquiring data to elucidate and quantify the propensity of amino acids to interact with heme (HEM, HEC, SRM, VEA/VER) in its binding environment. This study focused on potential interactions with the entire heme molecule, including the porphyrin ring and attached groups; therefore, any amino acids with potential interactons with the heme iron, porphyrin ring, or groups on the porphyrin ring (e.g. vinyl, propionate groups), were included in the data gathered for this section. A potentially interacting amino acid was therefore defined as any amino acid with at least one atom within the distance cutoffs (5 and 7 Angstroms (A)) from the heme *molecule*.

Amino acid frequencies were obtained for residues within the distance cutoffs of 5A and 7A - these data are overlaid in several figures in Appendix A.1. The trends in these data are very similar and therefore only the data pertaining to the 7A distance cutoff are discussed below.

2.1.1 Heme-b

Amino Acid Frequencies in Binding Pocket

Figure 2.1 plots the frequency of each residue within 7A of heme-b.

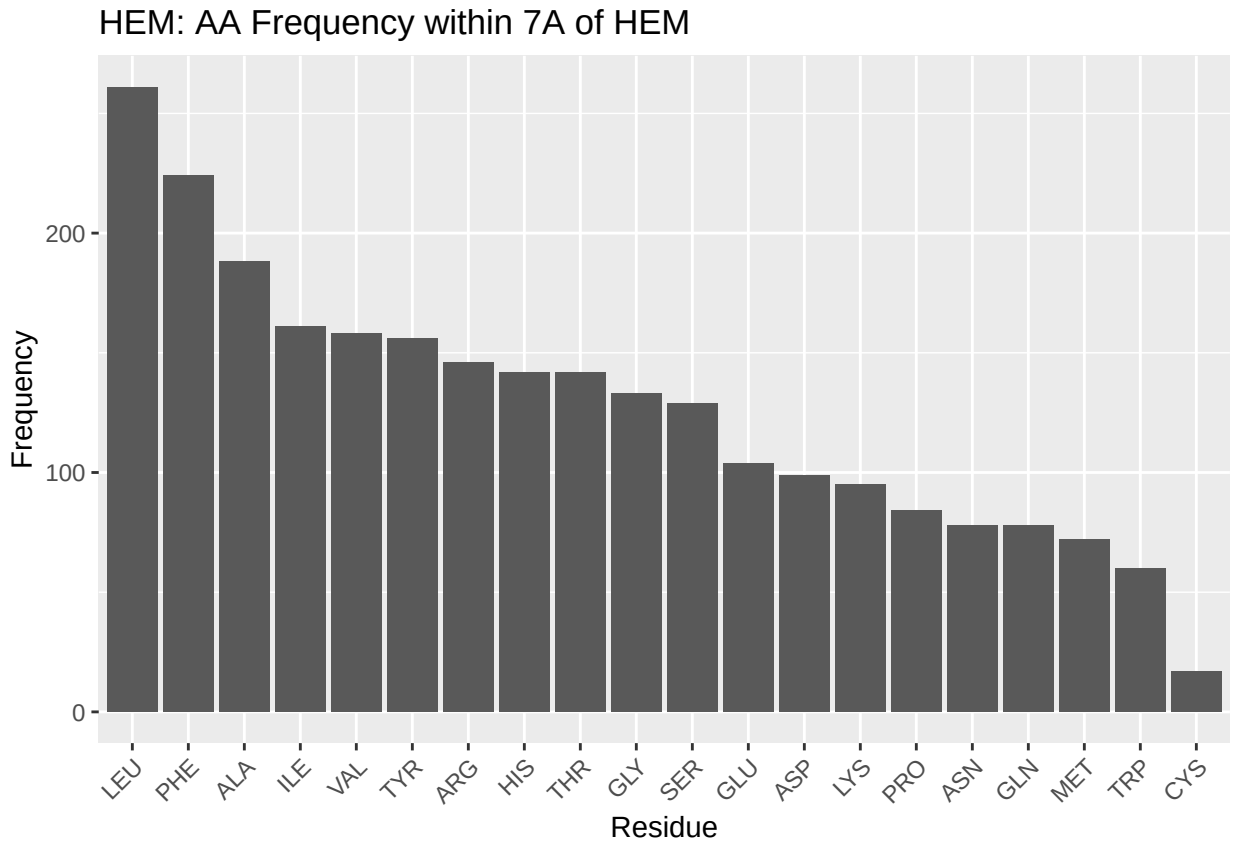

Figure 2.1: HEM: AA Frequency within 7A

Table 2.1: HEM: AA Frequency Table within 7A

Residue	Freq
LEU	261
PHE	224
ALA	188
ILE	161
VAL	158
TYR	156
ARG	146
HIS	142
THR	142
GLY	133
SER	129
GLU	104
ASP	99
LYS	95
PRO	84
ASN	78

Table 2.1: HEM: AA Frequency Table within 7A *(continued)*

Residue	Freq
GLN	78
MET	72
TRP	60
CYS	17

Beginning at the left of Figure 2.1 and moving right, large, nonpolar amino acids appear most frequently within 7A: LEU and PHE; ILE appears less frequently than these two amino acids but nonetheless is in high frequency. Small, nonpolar amino acids ALA and VAL also appear very frequently. As the majority of the heme-b molecule is made up of the nonpolar porphyrin ring, these amino acids are therefore likely in such high frequency to provide the nonpolar interactions with the pyrole groups and methyl and vinyl groups.

Tyrosine, arginine, histidine appear next most frequently. The two propionate groups on heme make polar interactions with salt bridges formed between arginine groups within the binding environment[8]. Therefore, the tyrosine and histidine likely form polar interactions with the portion of the propionate groups not interacting with the arginine salt bridges. This, in addition to the nonpolar interactions above, likely provides as hospitable of a binding environment as possible to coordinate the heme. It should be noted histidine is one of the residues that coordinates the iron atom, and this may therefore increase its frequency in the binding pocket.

Glycine is a small residue and cannot form significant interactions within its environment; however, its frequency, or lack thereof (compared to background frequency, discussed below), suggests the binding pocket may not require as much flexibility or spatial considerations as in the rest of the protein.

Next appear serine, glutamate (glutamic acid) and aspartate (aspartic acid) and lysine. These are polar residues, and glutamate and aspartate are negatively charged; lysine is polar too, but positively charged (at pH 7). The negative charge on glutamate and aspartate may explain why they are fairly infrequent: although polar, the negative charge may induce a repulsion effect with the propionate groups.

Or, it may be that other amino acids are preferable, as is likely the case for lysine. Lysine is polar and positively charged; but arginine residues forms the salt bridges necessary for propionate to make polar interactions. And histidine coordinates the heme iron. Therefore the infrequency of lysine may be less due to a problem with lysine and more due to a preference for other polar amino acids.

Proline is a small nonpolar amino acid in low frequency; the trend for heme-b, at least, appears to be to favor large nonpolar amino acids in the binding pocket. This may suggest that a large amount of nonpolar interactions, per residue, is favored in the binding pocket, perhaps because of the limited space available to position residues to interact with heme.

Asparagine and glutamine are both medium-sized polar amino acids; given the trends already discussed it is surprising these are not in greater abundance. But as with proline, it may simply be a matter of maximizing the benefit of the interactions that may be formed with the heme; while asparagine and glutamine are polar, amino acids like arginine and histidine are both polar and positively charged (and arginine forms salt bridges), capable of stronger interactions with the electronegative propionate groups.

Methionine and tryptophan appear very infrequently in the binding pocket. Tryptophan is very surprising to find as second-to-least frequent. It is a large nonpolar amino acid - but perhaps its single, potential hydrogen bond, although weak, is enough to prefer completely nonpolar residues. Or, with its size, it is preferable to have more numerous, smaller nonpolar residues that can favorably interact with the porphyrin while reducing steric hindrance of other residues in the environment. The reason for methionine's low frequency is not clear, perhaps for similar reasons as with proline, where more intensely nonpolar residues are preferred, rather than less nonpolar residues being unfavorable.

Cystine appears most infrequently of all the amino acids in the binding pocket. This is quite surprising - cystine is the other highly conserved residue that may coordinate the heme iron. Perhaps the sample of PDBs used in this study mostly use histidine to coordinate the iron - but this would only account for one residue in

the binding pocket per pdb. Therefore these results suggest that while cystidine may be well suited to coordinate the iron in heme, it is poorly suited to form any nonpolar interactions with the porphyrin ring, leaving the task up to other, more suitably, intensely nonpolar amino acids.

Moving away from discussing individual amino acid populations, what is especially notable of the data for heme-b is that nonpolar residues appear in much greater frequency than polar residues. Nonpolar interactions with heme are therefore more numerous than polar interactions. Their multiplicity may also suggest that they are potentially of greater importance than previously thought. At the very least, these results suggest that polar interactions and coordination of the iron atom, while necessary for heme binding, are insufficient, and that nonpolar interactions and the population of nonpolar residues in the binding pocket should be considered when examining the binding environment of heme.

Comparison with Background Amino Acid Frequencies

While the frequencies of amino acids in the binding pocket have been discussed, it may also be of interest to compare against the background amino acid frequency, the general frequency of amino acids within the entire monomer. The degree to which any results may affect the significance of the frequencies of the amino acids in the binding pocket is unclear - those amino acids are interacting with the heme. However, an in depth examination of similarities and differences may reveal that some amino acids may simply be extremely highly conserved by chance and by virtue of their numerous population, rather than some chemical benefit.

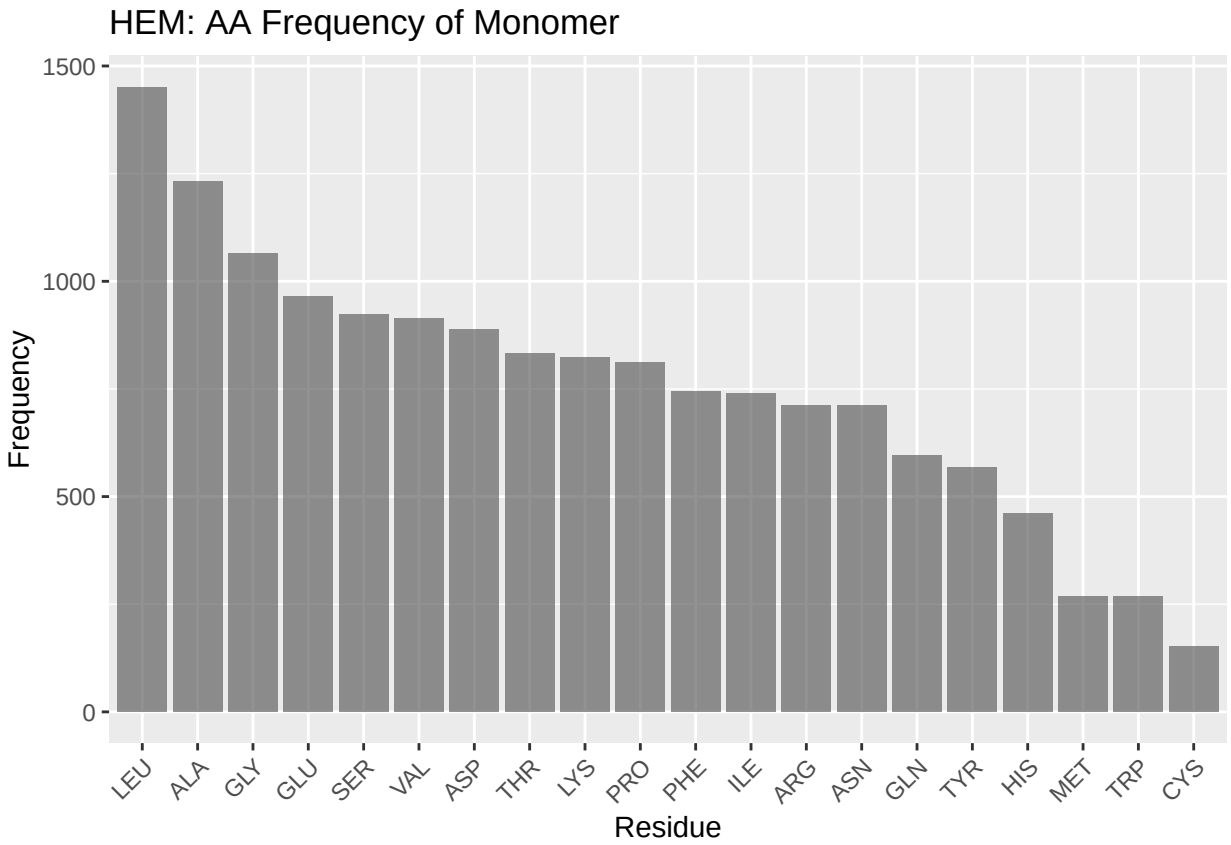

Figure 2.2: HEM: AA Frequency of Monomer

Figure 2.2 documents the frequencies of amino acids overall within the monomer.

Leucine and alanine, as in the binding pocket frequencies, are highly frequent in the overall monomer. This may suggest their prevalence in the binding pocket may simply be due to a high population of leucine and alanine in hemoproteins.

However, after these two amino acids the tendencies in frequency for the binding pocket and the monomer at large diverge. Glycine is in high frequency - likely due to more complex geometry e.g. helices outside the binding pocket. In interest of brevity, the remaining frequencies are summed up thus: the same trends that appear to exist in the binding pocket do not appear to exist in the monomer at large. While the order of frequencies in conserved binding pockets can be rationalized, justifying the overall frequencies in monomers invites significant speculation.

Distributon of Amino Acids by Distance

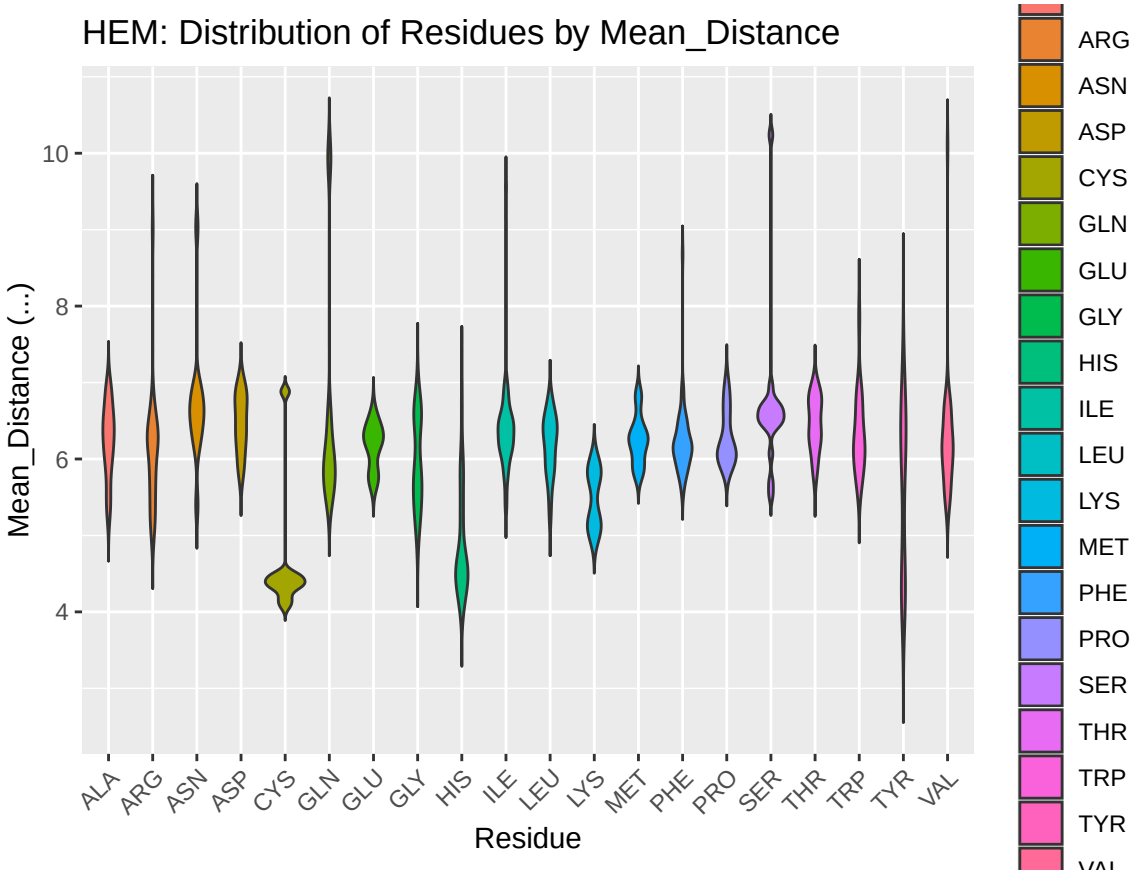

Figure 2.3: HEM: Residue Distribution by Distance

After an exhaustive exploration of the relative frequencies of amino acids in the binding pocket, Figure 2.3 below is fairly straightfoward. It plots the distribution of amino acids in the binding pocket against their distance from the iron of the heme.

We find that only a few residues come in close contact (<4A) of the heme: cysteine, histidine, and tyrosine. Most residues center their distribution at around 6A, although lysine seems more biased than the remaining residues to be a bit closer. Cysteine and histidine may be at least in part explained to be close due to their use as coordinating residues; histidine, being in greater frequency, may also be this close due to favorable interactions with the porphyrin ring.

The proximity of tyrosine however, is more notable. It cannot form coordination bonds with the heme iron, but tyrosine residues do interact with the propionate groups. Tyrosine is also required for redox reactions, and part of the population

of tyrosine residues may therefore be in close proximity to heme to facilitate electron transfer in various enzymes [1]. These results suggest that of all potentially interacting polar/positively charged residues, tyrosine is the most likely at least to be in close proximity to the heme molecule. Whether this illustrates an importance of tyrosine to interact with propionate groups, or instead the need for tyrosine to be in close proximity in order to form such interactions, or simply demonstrates involvement in oxidation/reduction reactions, is beyond the scope of this study.

2.1.2 Heme-c

Amino Acid Frequencies in Binding Pocket

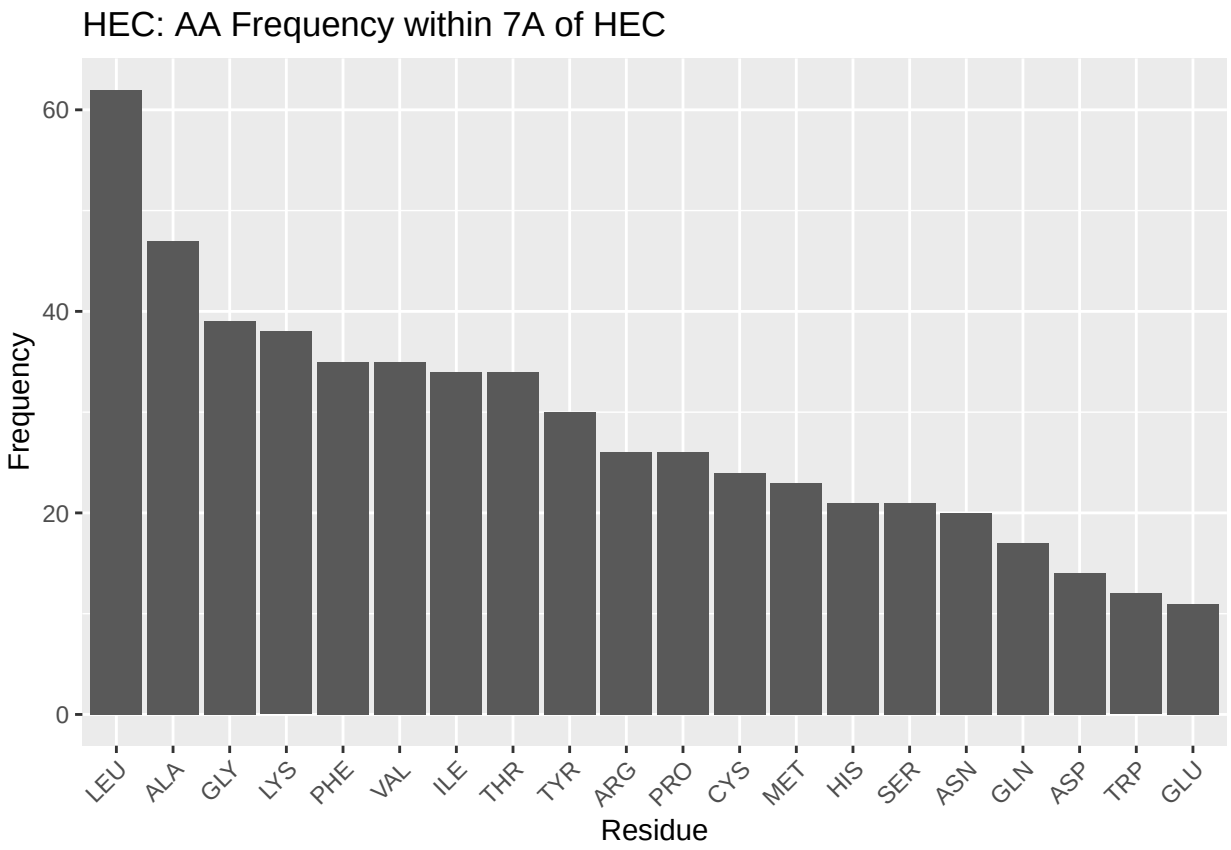

Figure 2.4: HEC: AA Frequency within 7A

Leucine and alanine again are highly frequent for HEC, followed by quite similar trends, and therefore HEC will not be as thoroughly discussed as HEM. The most notable differences may be that GLY and CYS are in far higher frequency than in heme. Heme-c almost always forms covalent bonds with cysteine residues, and

this may explain that frequency. But as for the high frequency of glycine, the reason for its abundance is unclear, although it seems it may have an important role in heme-c pockets.

Table 2.2: HEC: AA Frequency Table within 7A

Residue	Freq
LEU	62
ALA	47
GLY	39
LYS	38
PHE	35
VAL	35
ILE	34
THR	34
TYR	30
ARG	26
PRO	26
CYS	24
MET	23
HIS	21
SER	21
ASN	20
GLN	17
ASP	14
TRP	12
GLU	11

Comparison with Background Amino Acid Frequencies

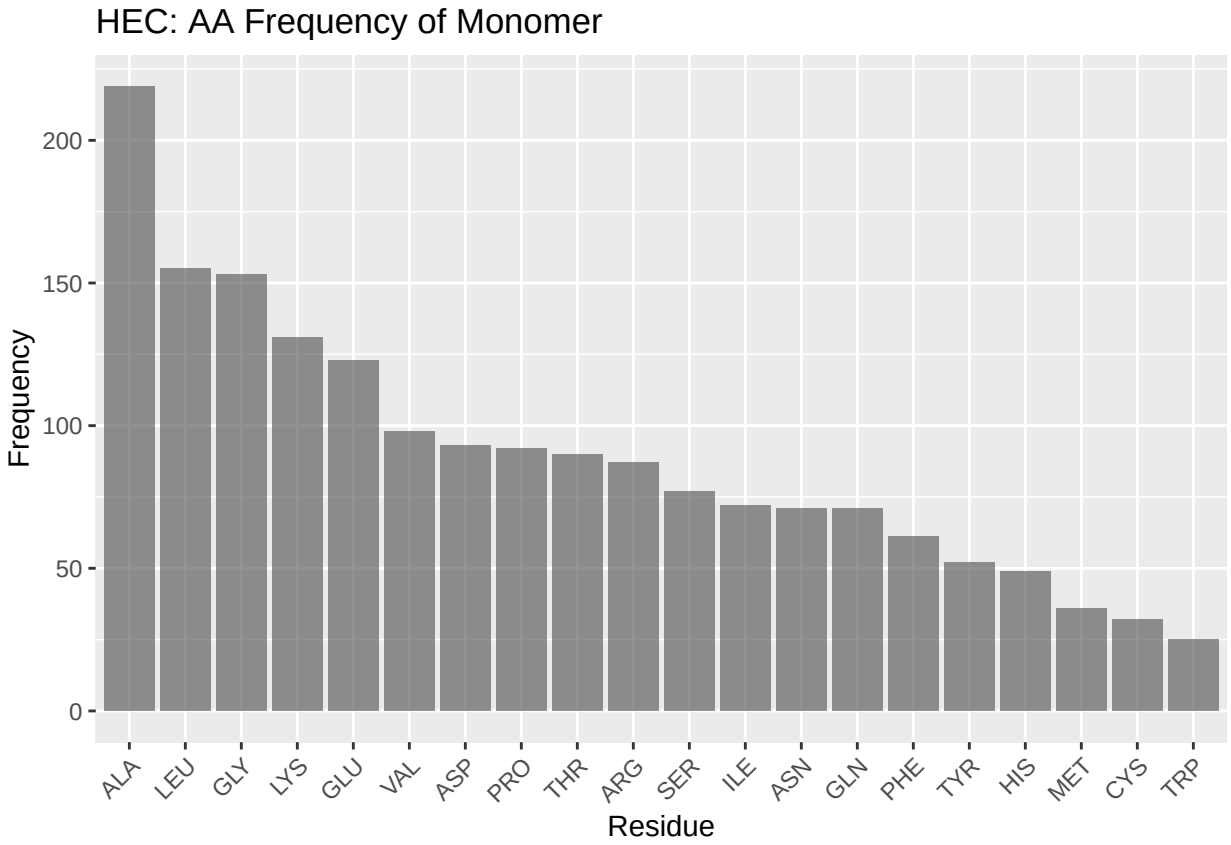

Figure 2.5: HEC: AA Frequency of Monomer

Generally, the heme-c monomer AA frequency profile appears similar to the heme-b monomer, with a high frequency of alanine and leucine, followed by a divergence in the frequency of amino acids and therefore a struggle to form any meaningful discussion when it comes to comparing the binding pocket frequencies against background frequencies.

Distributon of Amino Acids by Distance

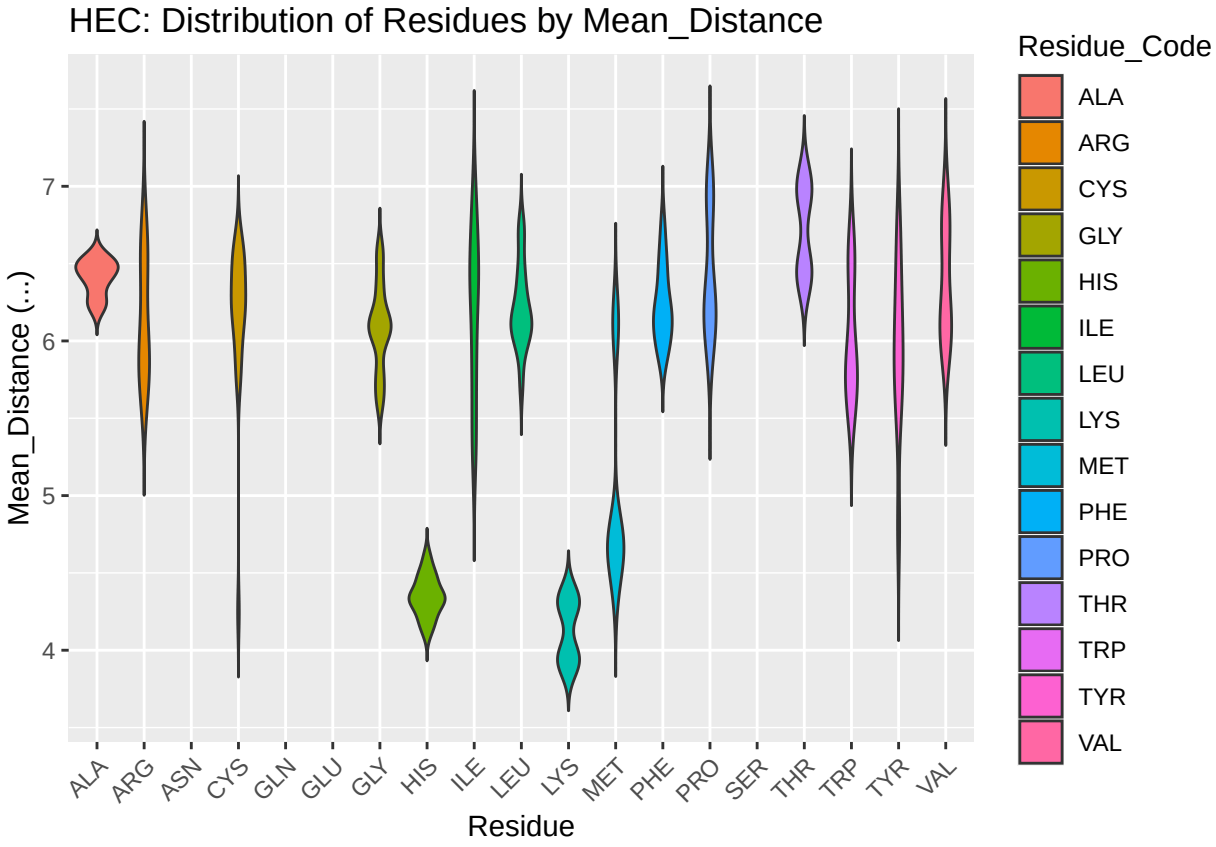

Figure 2.6: HEC: Residue Distribution by Distance

The distribution of amino acids over distance from the heme iron for HEC is similar to HEM, with some exceptions. Cys, His, Tyr again are amongst the closest residues to HEC, likely for the same reasons of very strong polar interactions or coordination. Additionally, cysteine forms covalent, thioether bonds with heme-c, providing further justification for its proximity. However, for heme-c, lysine and methionine also are very proximal. The methionine residues are nonpolar, small, neutral; lysine is polar and positively charged; neither of these residues are favored to be included in the heme-b binding environment despite very similar structures. The reason for their inclusion so close to the binding pocket is therefore unclear, but based on their distribution, and lysine being even more close proximity than heme, the results suggest these two residues may have important roles.

2.1.3 Verdoheme

Amino Acid Frequencies in Binding Pocket

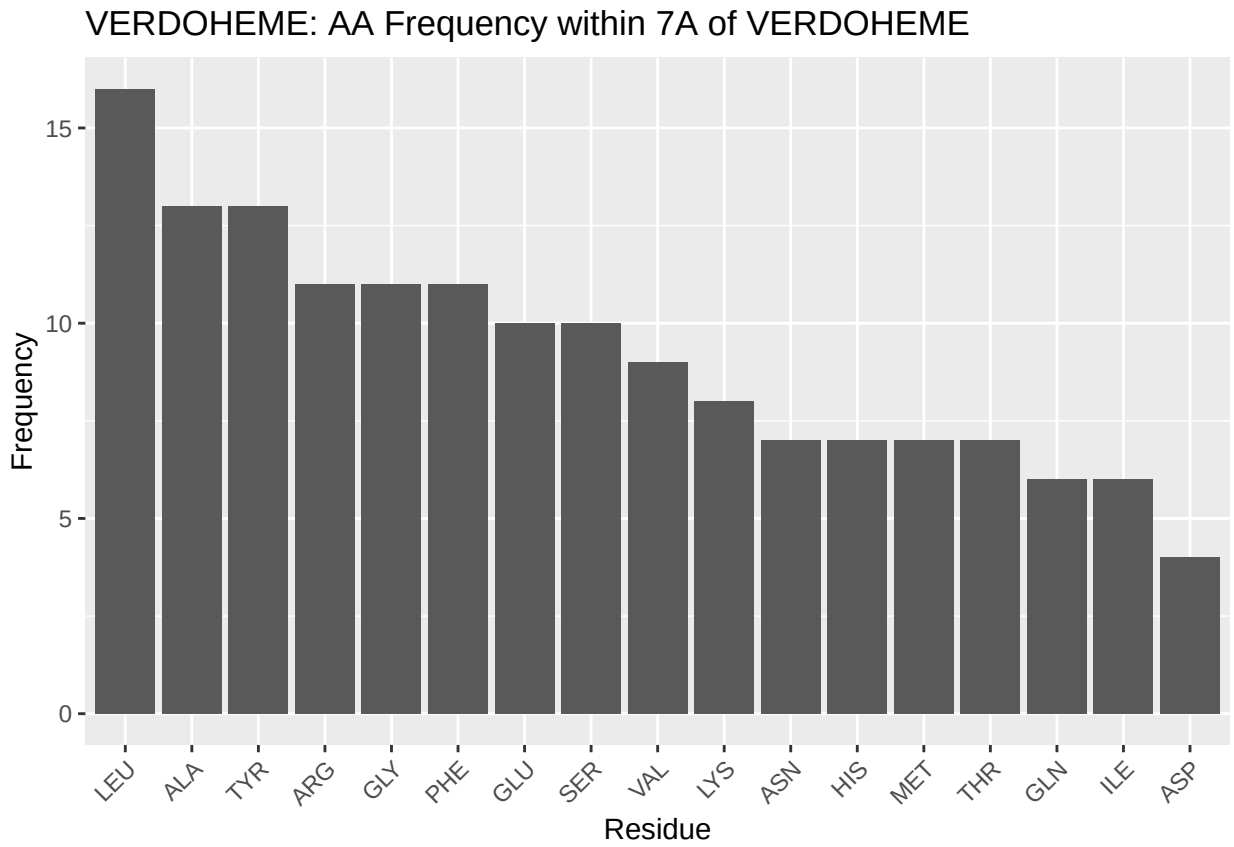

Figure 2.7: VERDOHEME: AA Frequency within 7A

Table 2.3: VERDOHEME: AA Frequency Table within 7A

Residue	Freq
LEU	16
ALA	13
TYR	13
ARG	11
GLY	11
PHE	11
GLU	10
SER	10
VAL	9
LYS	8
ASN	7
HIS	7
MET	7

Table 2.3: VERDOHEME: AA Frequency Table within 7A *(continued)*

Residue	Freq
THR	7
GLN	6
ILE	6
ASP	4

The frequqency of amino acids in the binding pocket for verdoheme is dissimilar from heme-b and heme-c above. This is fairly surprising, given that verdoheme is an intermediate in the binding pocket for heme-b within heme oxygenases.

Leucine and alanine are again most frequent, but after these, results diverge. Tyrosine and arginine are next most frequent - surprising, given that this is still the same pocket that bound heme-b. The data for heme-b indicate more frequent nonpolar residues before tyrosine. Chemically, it may be that as heme-b is oxidized, there is greater need for polar interactions; this would help to explain the high frequency of polar residues, but does not explain the shift in amino acid frequencies within what would be expected to be a similar binding pocket - all verdoheme PDBs in this in study were sourced from heme oxgenase proteins. Some heme oxygenases are included for heme-b, but they are amongst a diverse set of proteins. Therefore, the heme oxygenase environment may simply be host to more polar residues than normal for hemoproteins. This also agrees with tyrosine's inclusion in redox reactions, and it may be favored to be present in heme oxygenase. These results indicate more about the heme oxygenase environment than the verdoheme binding environment - however, these two are inseparable, given verdoheme only appears in heme oxygenase. A dedicated investigation to the heme binding environment for heme oxygenase, may therefore be warranted in future study.

Glycine is the next most frequent - it is in lower frequency, relatively, for heme-b. As with other heme molecules, it is not clear as to what the role of glycine is in binding verdoheme.

Comparison with Background Amino Acid Frequencies

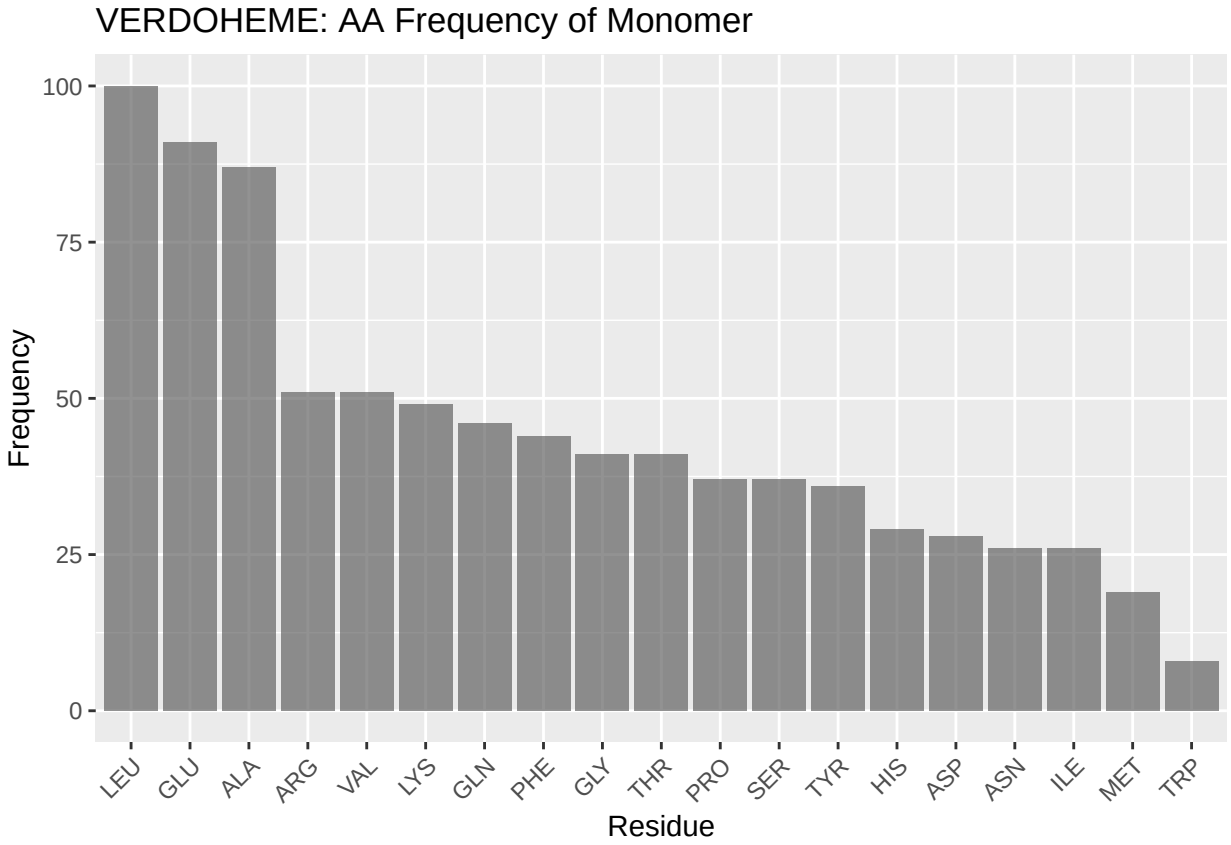

Figure 2.8: VERDOHEME: AA Frequency of Monomer

Besides the frequencies of leucine and alanine, which have been found for heme-b and heme-c above to be highly frequent in hemoproteins at large, the frequency profiles for the verdoheme binding environment and monomers is shown to be quite dissimilar, supporting the results for the binding environment as unique, not simply due to background frequency.

Distributon of Amino Acids by Distance

The low sample size for verdoheme leads here to a poor figure with few residues plotted. This is likely attributable to an insufficient amount of distances and residues to cross-reference against each other, an operation that successfully occurs for all similar graphs. Regardless, the data that are plotted will be discussed.

The highly conserved histidine for hemoproteins is exclusively within 5A for verdoheme. This result again suggests that at least some of the data for verdoheme

may be highly biased because of the small sample size - heme-b data included a greater range for histidine. Or, perhaps for heme oxygenases heme is solely present to coordinate the iron atom, leading to all His residues being nearby verdoheme. The close proximity of glycine to verdoheme is also unexpected and unable to be explained without further study. The remainder of the residues plotted appear to follow the trends seen in for the other types of heme, with distance values centered around 6A and unremarkable distributions.

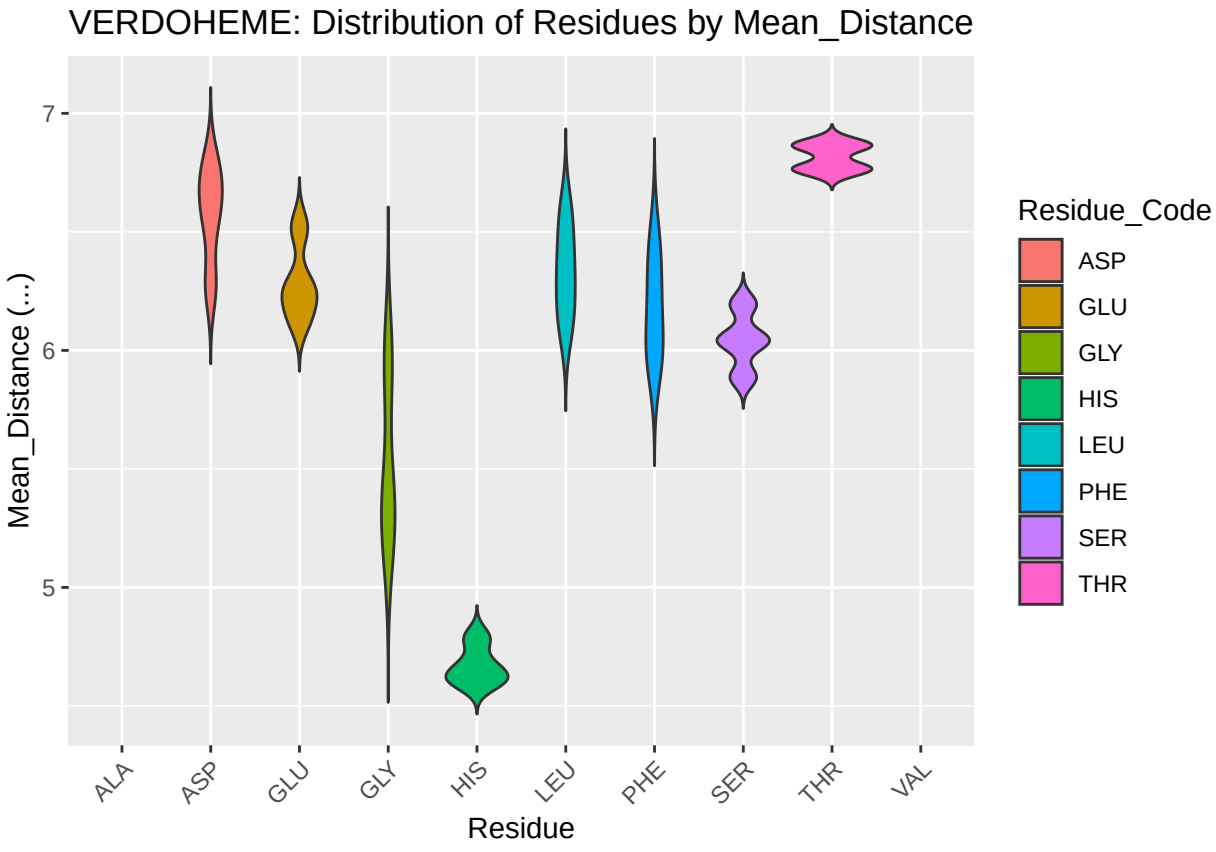

Figure 2.9: VERDOHEME: Residue Distribution by Distance

2.1.4 Siroheme

Amino Acid Frequencies in Binding Pocket

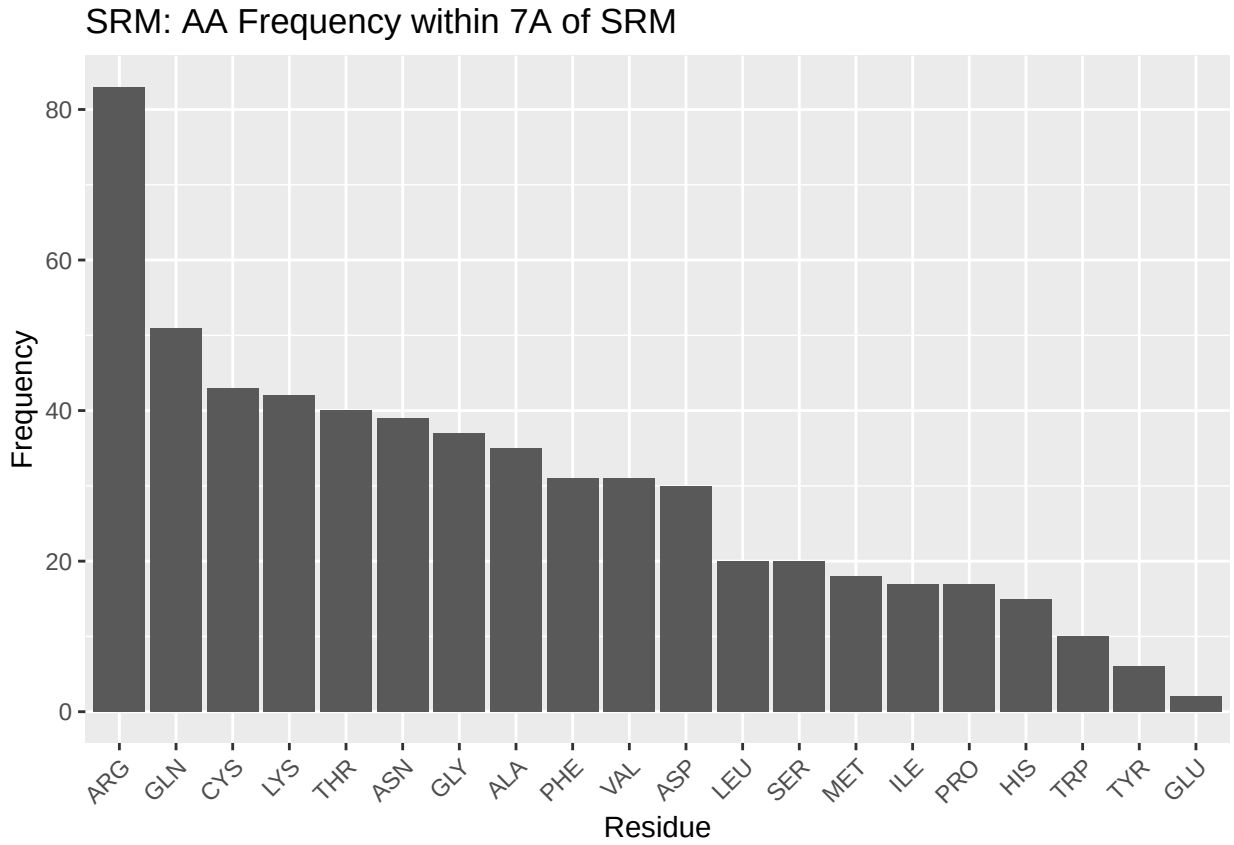

Figure 2.10: SRM: AA Frequency within 7A

Table 2.4: SRM: AA Frequency Table within 7A

Residue	Freq
ARG	83
GLN	51
CYS	43
LYS	42
THR	40
ASN	39
GLY	37
ALA	35
PHE	31
VAL	31
ASP	30
LEU	20
SER	20

Table 2.4: SRM: AA Frequency Table within 7A *(continued)*

Residue	Freq
MET	18
ILE	17
PRO	17
HIS	15
TRP	10
TYR	6
GLU	2

Siroheme, with a structure highly dissimilar to the other heme molecules examined, should be expected to have a different amino acid frequency profile – and indeed we confirm this in our results.

Nonpolar residues are not the most abundant in the siroheme binding pocket. In fact, disproportionately frequent to the rest of the residues in the binding pocket is arginine. Siroheme is saturated with carboxyl and propionate groups; the entire porphyrin ring surrounded by polar, electronegative groups. And therefore a polar, positively charged amino acid such as arginine is reasonable to expect in the binding pocket – what is striking, however is the extreme preference for arginine; such a profile does not exist for the other types of heme. This can be at least explained; siroheme contains propionate groups that likely still form polar interactions with arginine salt bridges, and the carboxyl groups may also form polar interactions with arginine, therefore highly favoring arginine's presence in the binding pocket.

Arginine is followed by other polar amino acids: glutamine, cystine, lysine, threonine, and asparagine; a more homogenous trend than seen for the other heme molecules, in that the trend is not interrupted by residues of opposing polarity as for other types of heme. Though these results could be expected, they demonstrate the extent to which siroheme's binding pocket is dominated by polar residues. The preference for arginine out of all polar amino acids may be attributed to its positive charge, and ability to form salt bridges that interact with the propionate groups; lysine also has a positive charge and is polar, but does not form salt bridge interactions with the propionate groups. Cysteine is used to coordinate the iron of

siroheme, and while this did not significantly affect the frequency for other heme molecules, it is still possible this increases the value for cysteine for siroheme.

After this group of polar amino acids, glycine is the next most frequent. Glycine has been situated at about a median frequency for other heme molecules, so perhaps its frequency here, slightly above the median, is of note. Again, for glycine in particular, the reason for its particular frequency cannot be determined from this data, but it appears to have some role.

Finally we come to several nonpolar amino acids: alanine, phenylalanine, and valine. These amino acids define roughly the median of the frequency data. With all the polar groups on siroheme, it might be expected that only polar interactions would be desirable. However, the not minuscule frequency of these residues suggests nonpolar interactions still occur in the binding pocket; the porphyrin ring remains, as well as some methyl groups.

After these nonpolar residues the remaining frequencies do not follow a clear trend but regardless are discussed. After aspartate the remaining frequencies are considerably lower. This may be an artefact of a small sample size, or may suggest the remaining residues form, if any, far less favorable interactions with the heme.

Aspartate appears next most frequently; it is a polar, negatively charged amino acid (at pH 7). Siroheme is saturated with other electronegative groups; perhaps there is some repulsion between these groups and aspartate – this could explain why, despite being a polar residue, arginine does not appear very frequently in the binding pocket.

Leucine is the first of the residues of diminished frequency. It is nonpolar. It, and, skipping a frequency, methionine, isoleucine, and proline, appear less frequently, and therefore are likely disfavored from forming the relatively few nonpolar interactions that do occur. Why is not clear - other small, nonpolar residues, and other lengthy nonpolar residues appear in the pocket in greater frequency.

Serine appears just less frequently than leucine, and in this context may likely be considered a polar residue that is not as strongly polar or positively charged and

therefore less preferred to include in the binding pocket to form polar interactions with siroheme as other residues.

Histidine appears quite infrequently. As with siroheme, other, more strongly polar and perhaps less bulky residues are likely preferred.

Tryptophan is the least frequent nonpolar residue. The presence of a weak hydrogen bond and its size may preclude its inclusion in the binding pocket in lieu of more uniformly nonpolar residues that take up less space and can better form interactions with the few nonpolar areas of siroheme.

Tyrosine and glutamate are the least frequent polar residues. This is in stark opposition to the other heme molecules - tyrosine seemed to be favored for other heme molecules to form interactions with the propionate groups. Glutamate is also extremely infrequent, even in spite of its similarity to aspartate. Both are electronegative at pH 7 - glutamate's extra carbon may provide sufficient steric hindrance to render it less favored. In either case, the infrequency of these residues and the tendencies of other, more intensely polar or nonpolar amino acids to be more populous, suggests tyrosine and glutamate, in the siroheme binding environment, do not interact strongly enough to be favored over other polar residues.

Comparison with Background Amino Acid Frequencies

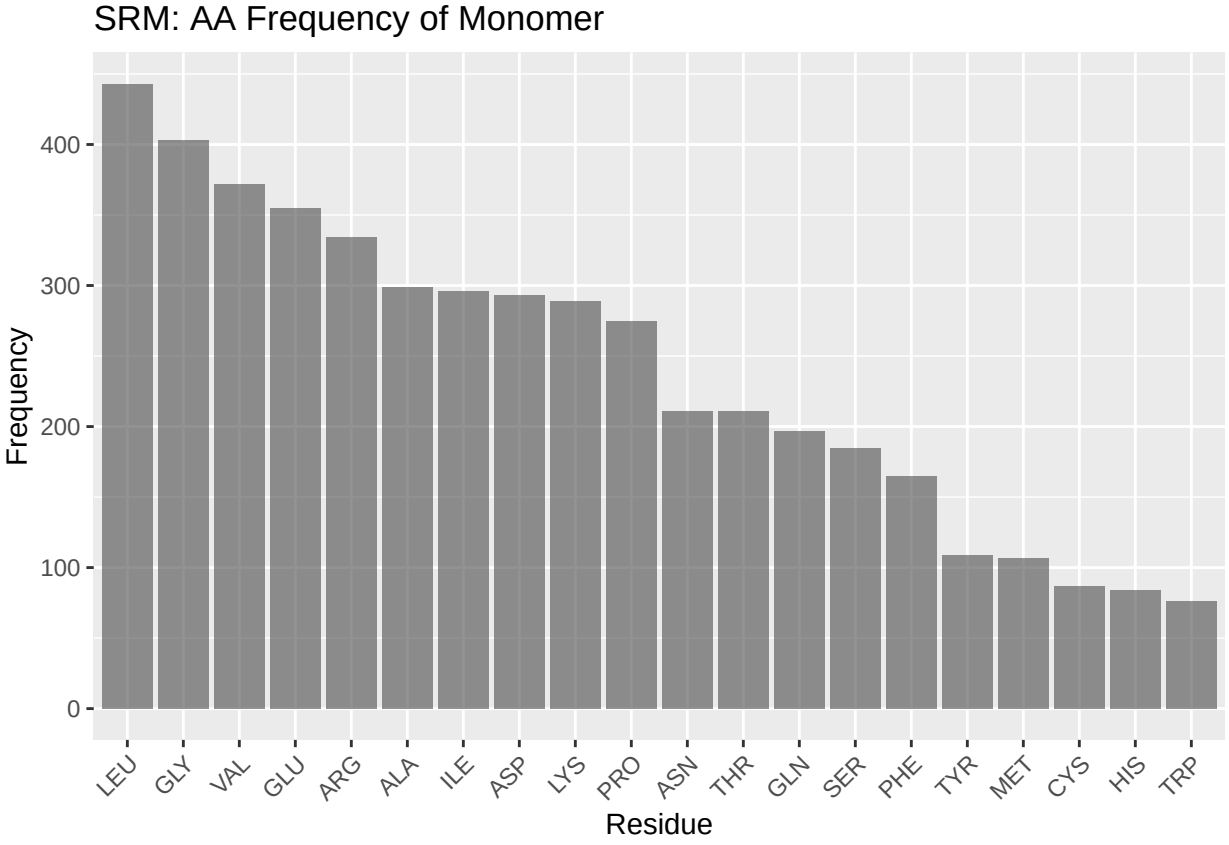

Figure 2.11: SRM: AA Frequency of Monomer

Compared to the other heme molecules, siroheme's binding pocket amino acid frequencies are even more different than the background frequencies. Arginine is far and away the most frequent amino acid in the binding pocket; leucine is the most populous amino acid in the monomer overall, seeming to follow a trend amongst the hemoproteins examined so far. Again, discussing the remainder of the frequencies of the monomer would be conjecture, but it is worthwhile to note that the pocket frequencies appear unique against the background.

Distributon of Amino Acids by Distance

Residues appear less uniformly distributed over distance for siroheme binding pockets when compared against the distribution for other heme molecules. Cysteine is the only residue that comes within 5A of siroheme; it is used to coordinate

the iron in siroheme, so this result is expected. The lack of other residues being within 5A, differing from other heme molecules, suggests the many carboxyl and propionate groups on siroheme prevent, or preclude the need for closer interaction except for coordinating residues.

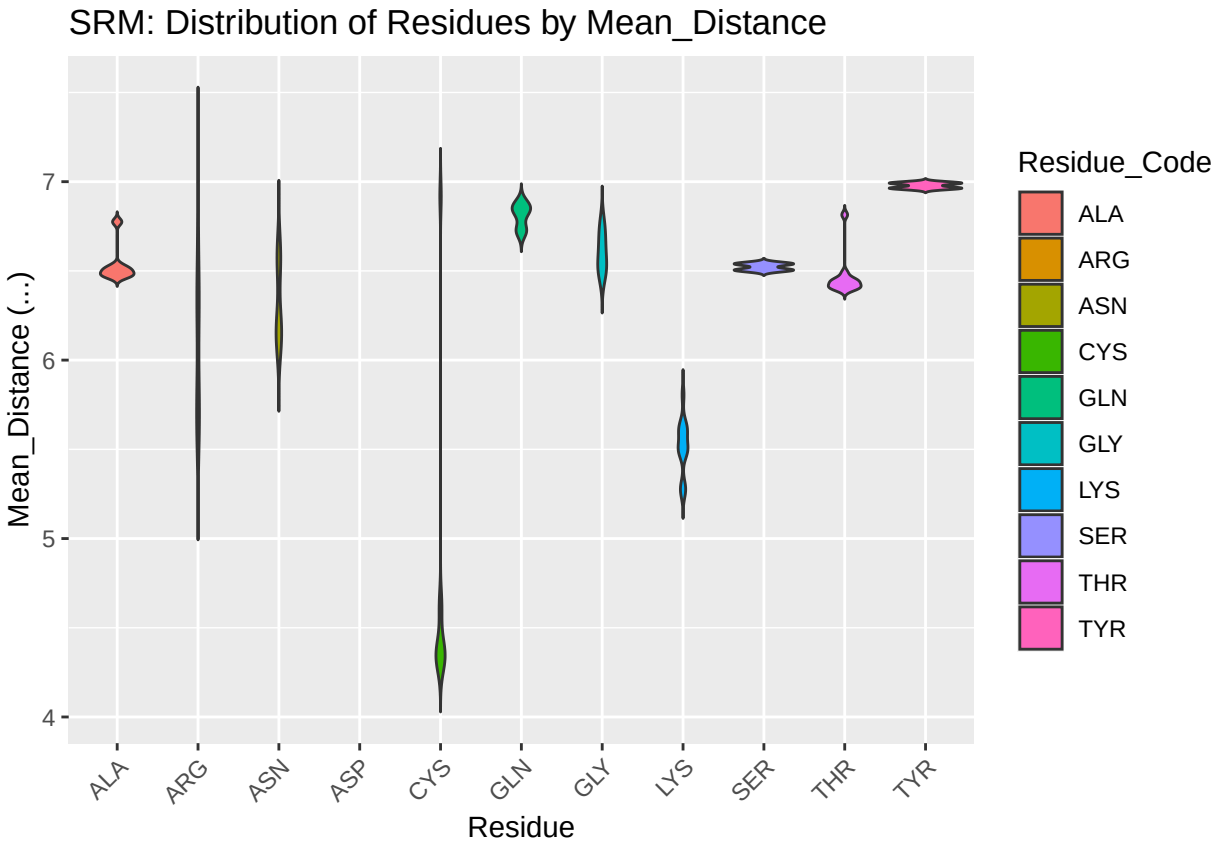

Figure 2.12: SRM: Residue Distribution by Distance

2.2 Volume of Heme Binding Pockets

Figures are shown below.

Volume results were rather spread out, with close agreement only found for heme-b. In general, volume for all heme molecules regardless of distance cutoff centered at approximately 1200 A^3. This result may be useful in protein engineering efforts, especially for selection or design of binding pockets.

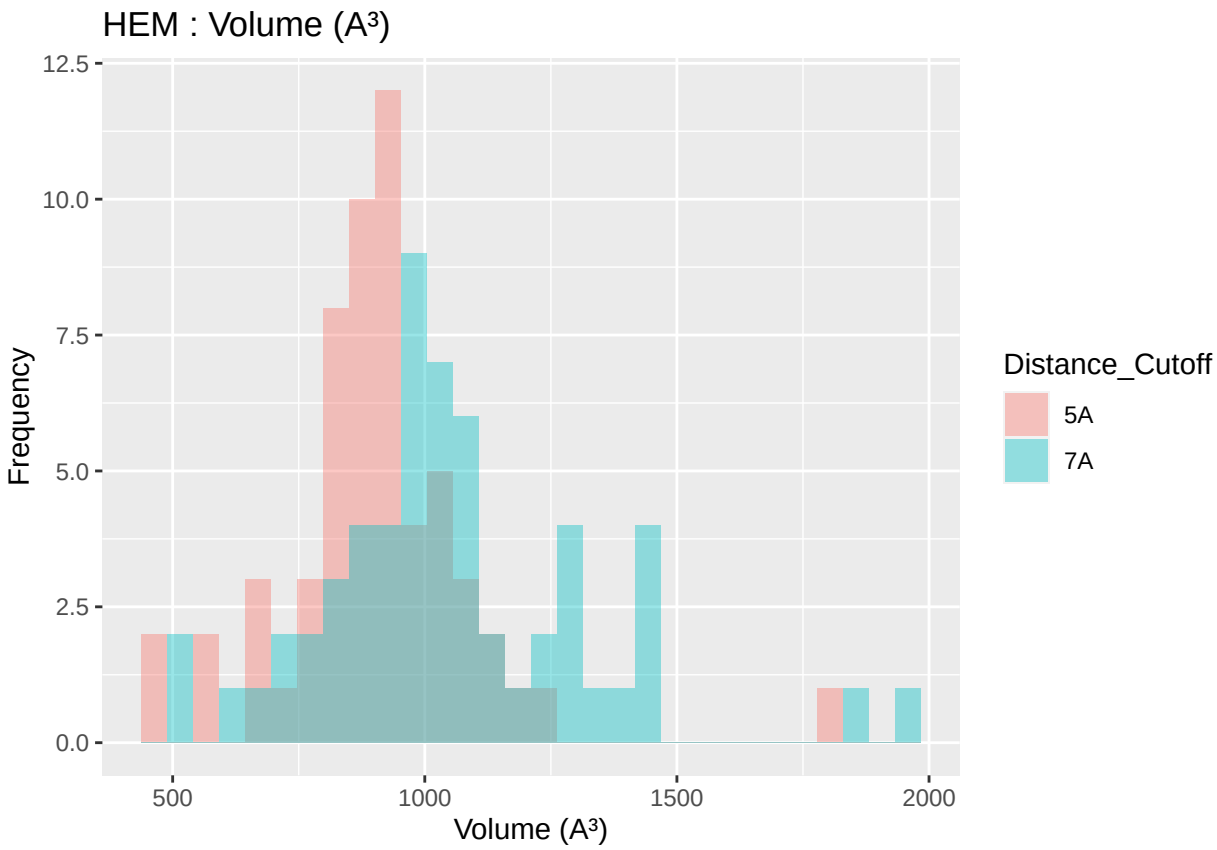

Figure 2.13: HEM: Volume of Binding Pocket

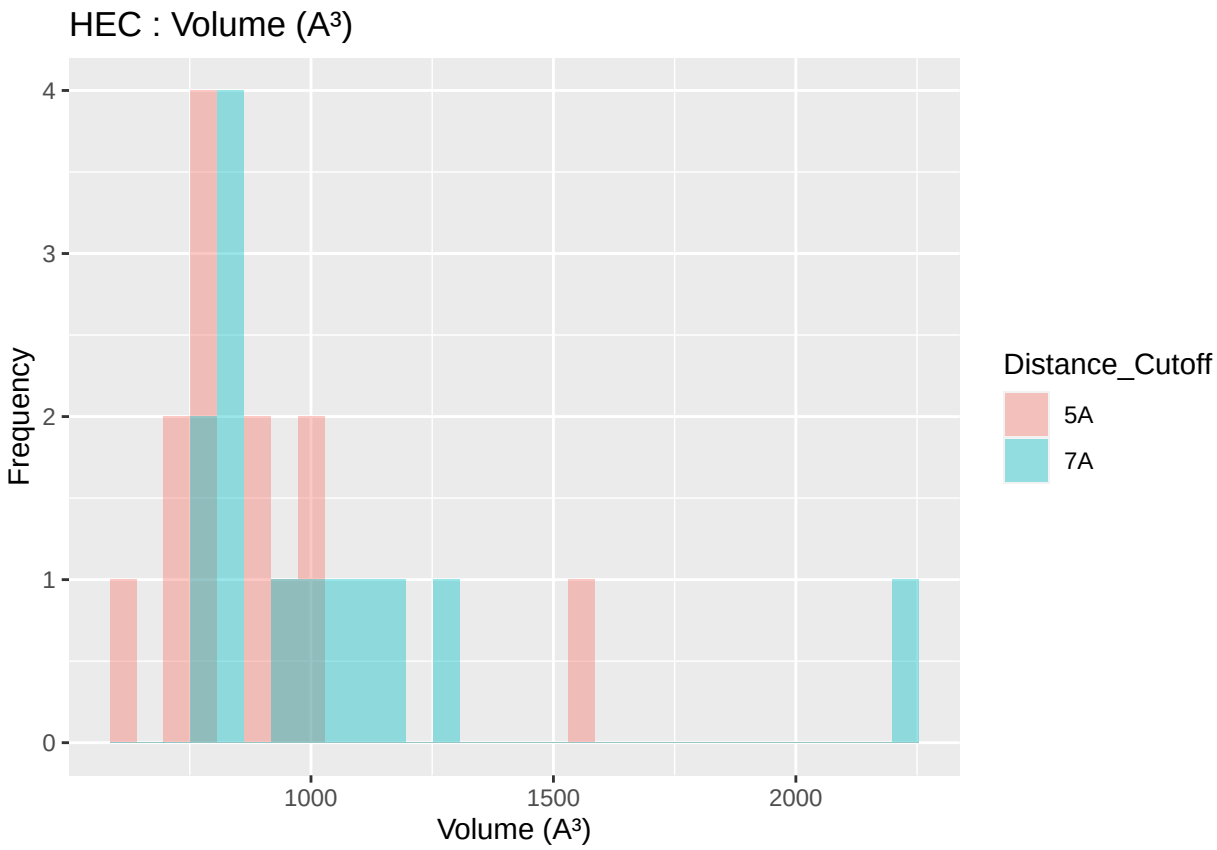

Figure 2.14: HEC: Volume of Binding Pocket

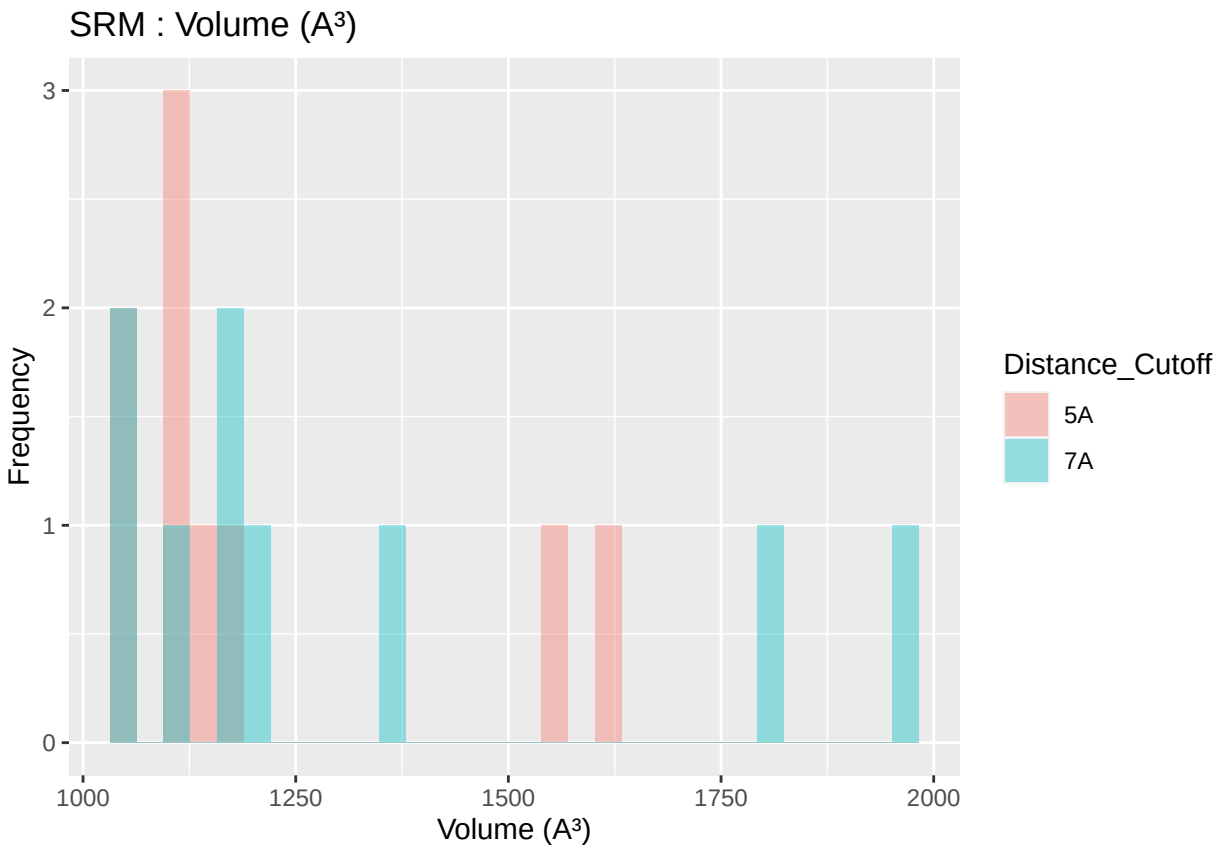

Figure 2.15: SRM: Volume of Binding Pocket

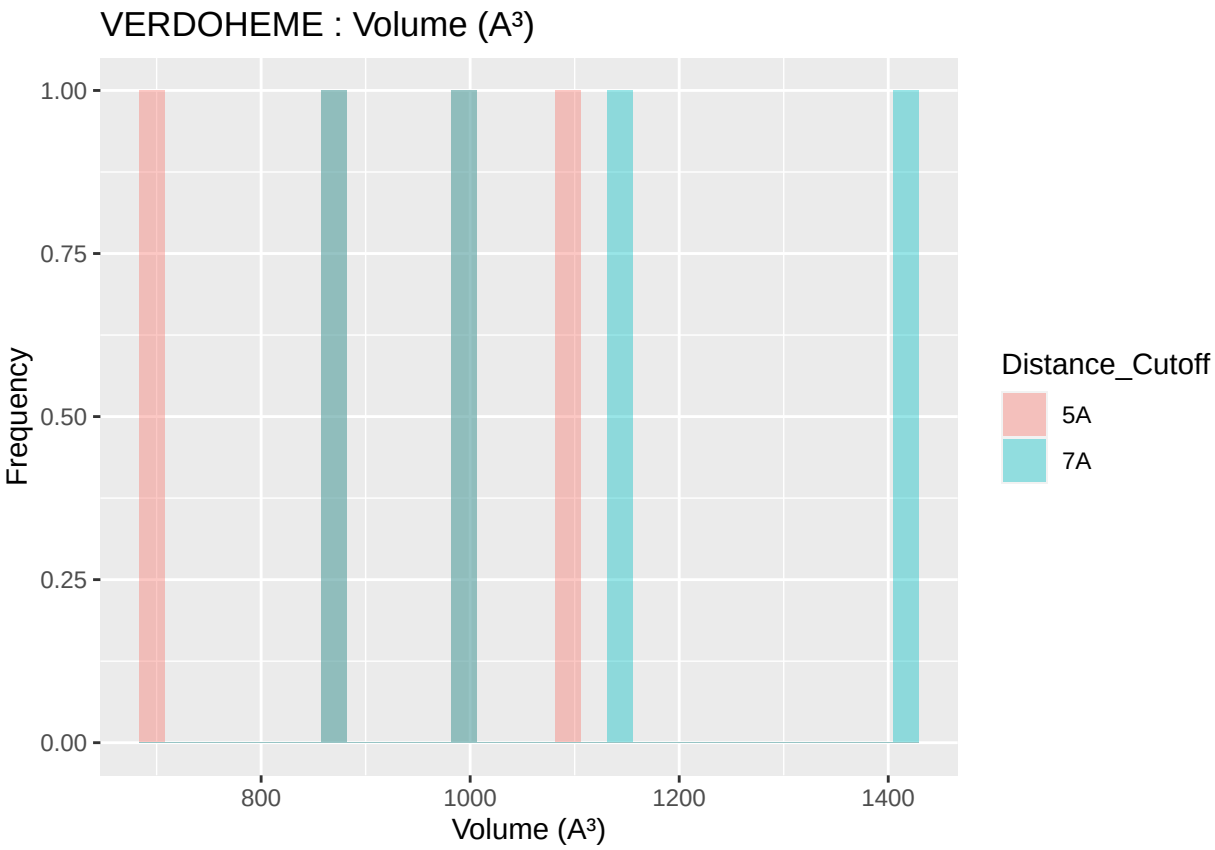

Figure 2.16: VERDOHEME: Volume of Binding Pocket

2.3 Surface Areas of Heme Molecules and Their Binding Pockets

2.3.1 Surface Area of Heme Molecules

Both solvent accessible and solvent excluded surface areas were calculated for heme molecules and binding pockets. The differences between these two measures were discussed in Section 1.3.3. The results are extremely similar for solvent accessible and solvent excluded surface areas; and therefore only solvent accessible surface area, a measure more practically interpreted into chemical phenomena, is discussed below. Figures and data for solvent excluded surface areas are available in Appendix A.2, A.3, and B.4. Solvent accessible surface area figures are shown below; data tables are available in Appendix B.4.

The solvent accessible surface area for all heme *molecules* themselves centers

around values of 1000 A². This result is reasonable, given the similarity in size and structure of all heme molecules, in spite of the attached groups. Figures are shown below; full data tables are available in Appendix B.4. The extreme outliers are likely artefacts of the method used to calculate surface area and potential conflicts with the method used to convert multimeric proteins to monomers.

2.4 Ligand Solvent Accessible Surface Area

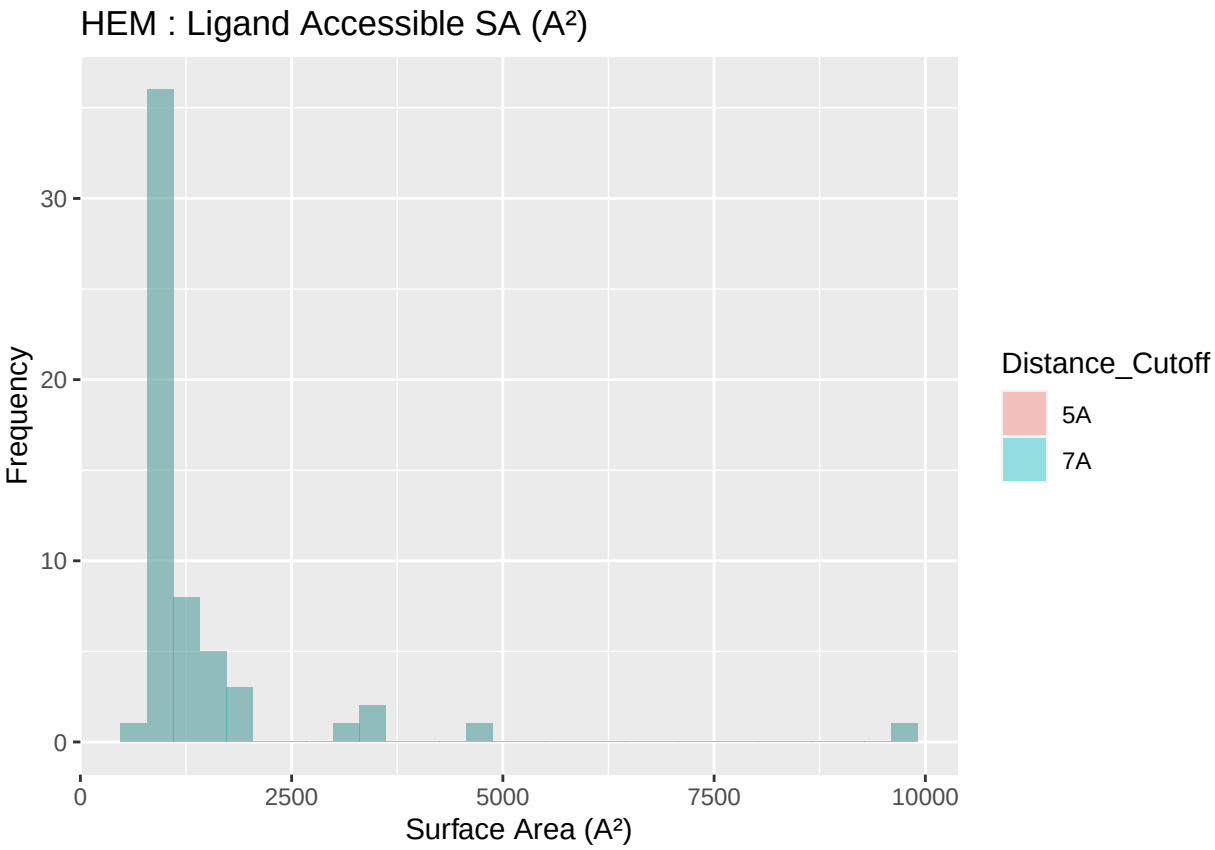

Figure 2.17: HEM: Ligand Accessible Surface Area

Figure 2.18: HEC: Ligand Accessible Surface Area

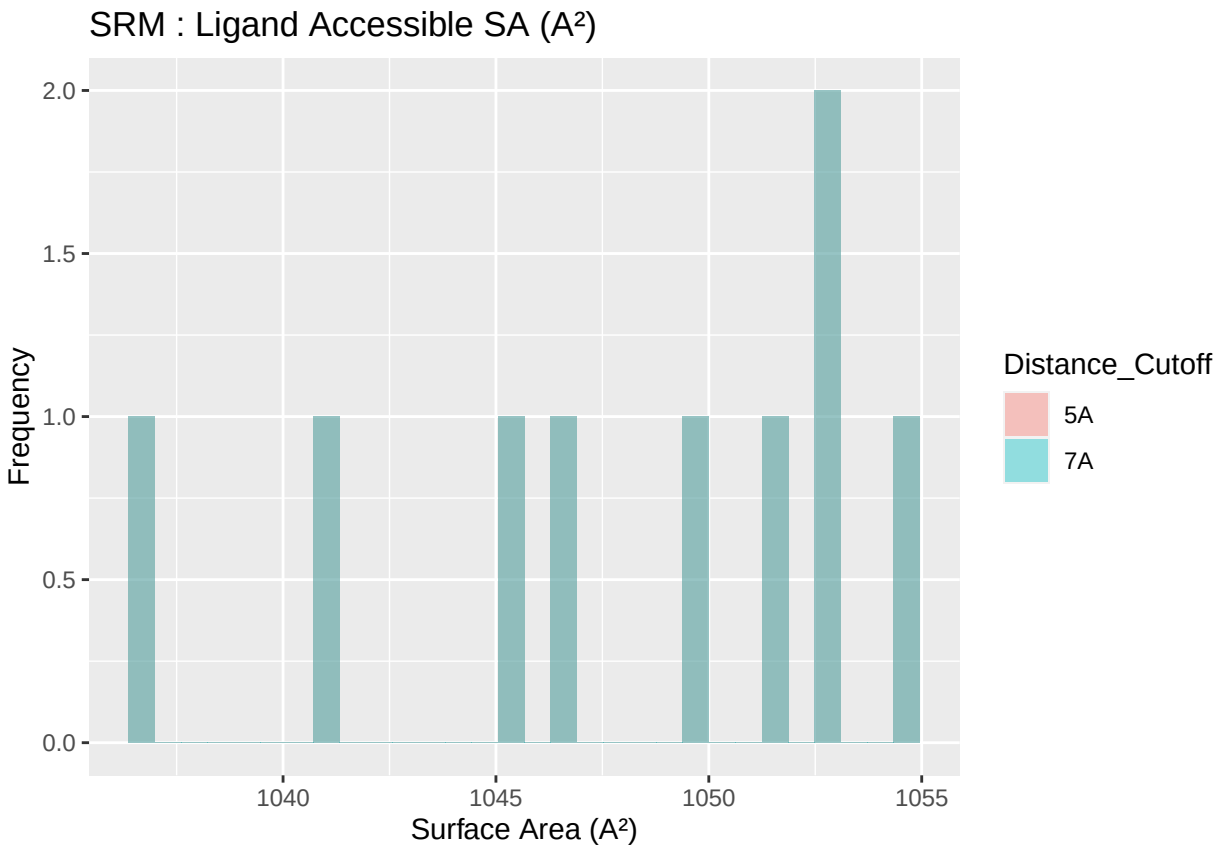

Figure 2.19: SRM: Ligand Accessible Surface Area

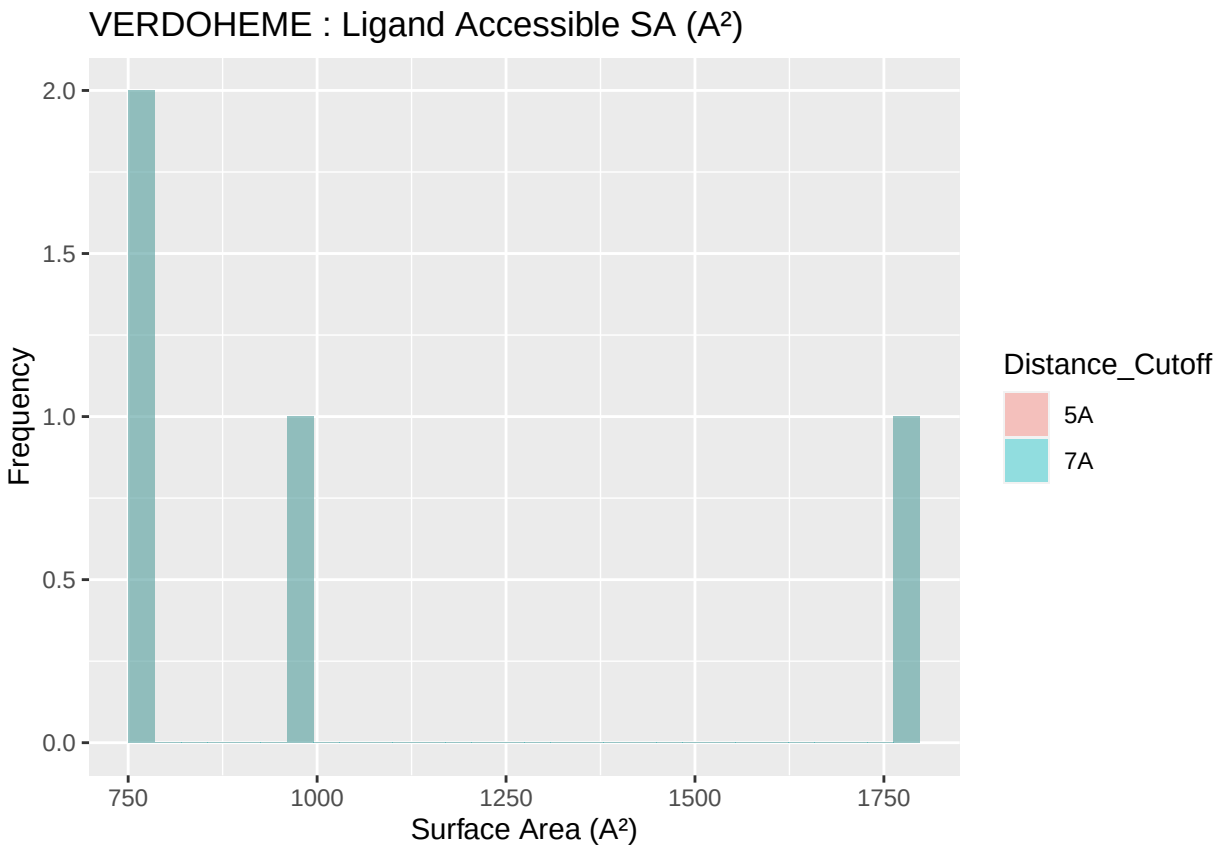

Figure 2.20: VERDOHEME: Ligand Accessible Surface Area

2.4.1 Surface Area of Binding Pockets

2.5 Pocket Solvent Accessible Surface Area

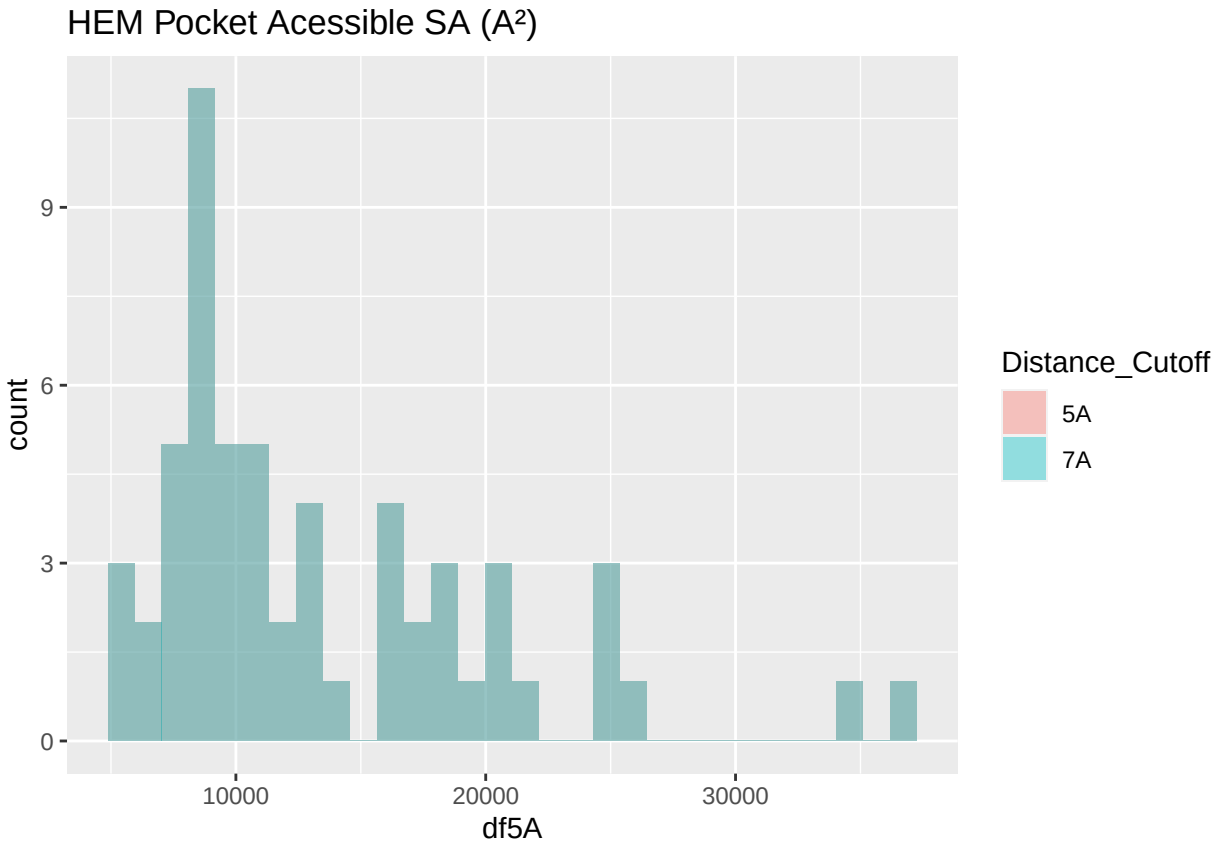

Figure 2.21: HEM: Pocket Accessible Surface Area

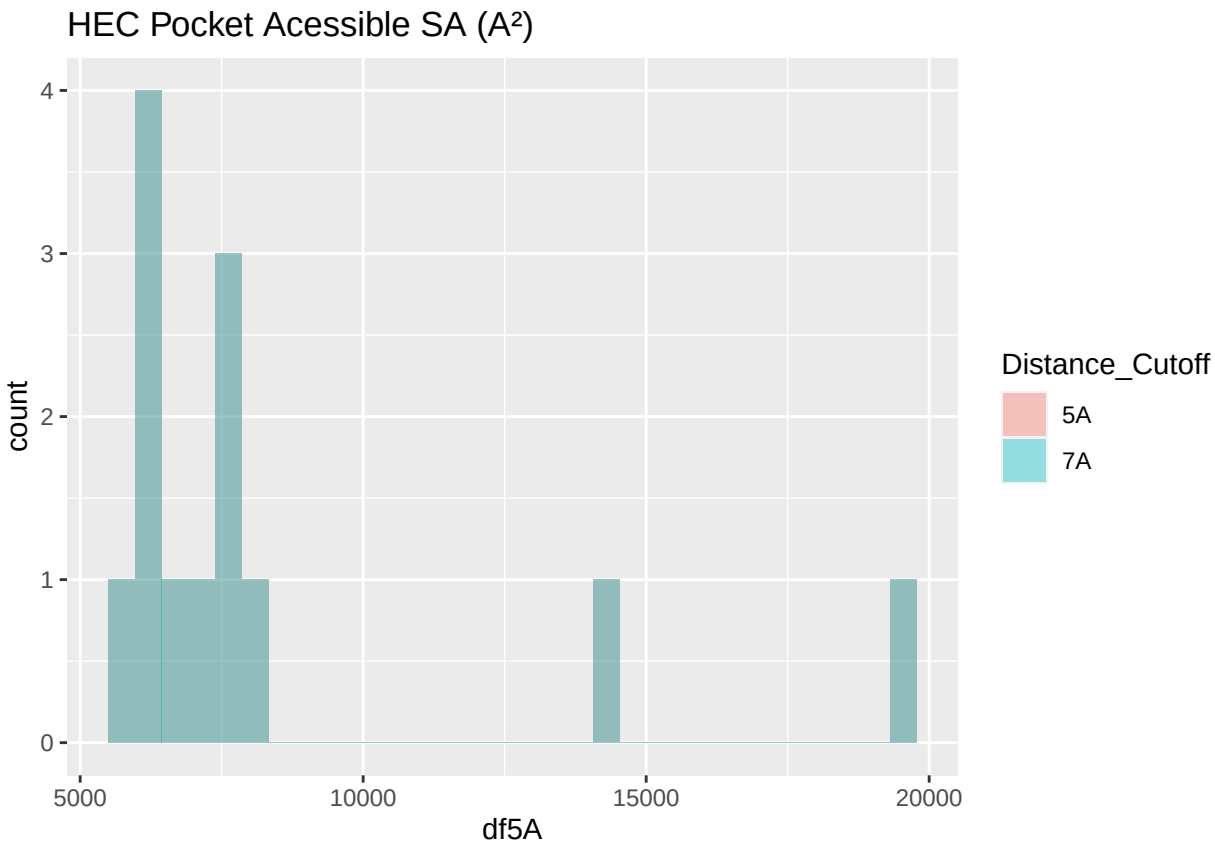

Figure 2.22: HEC: Pocket Accessible Surface Area

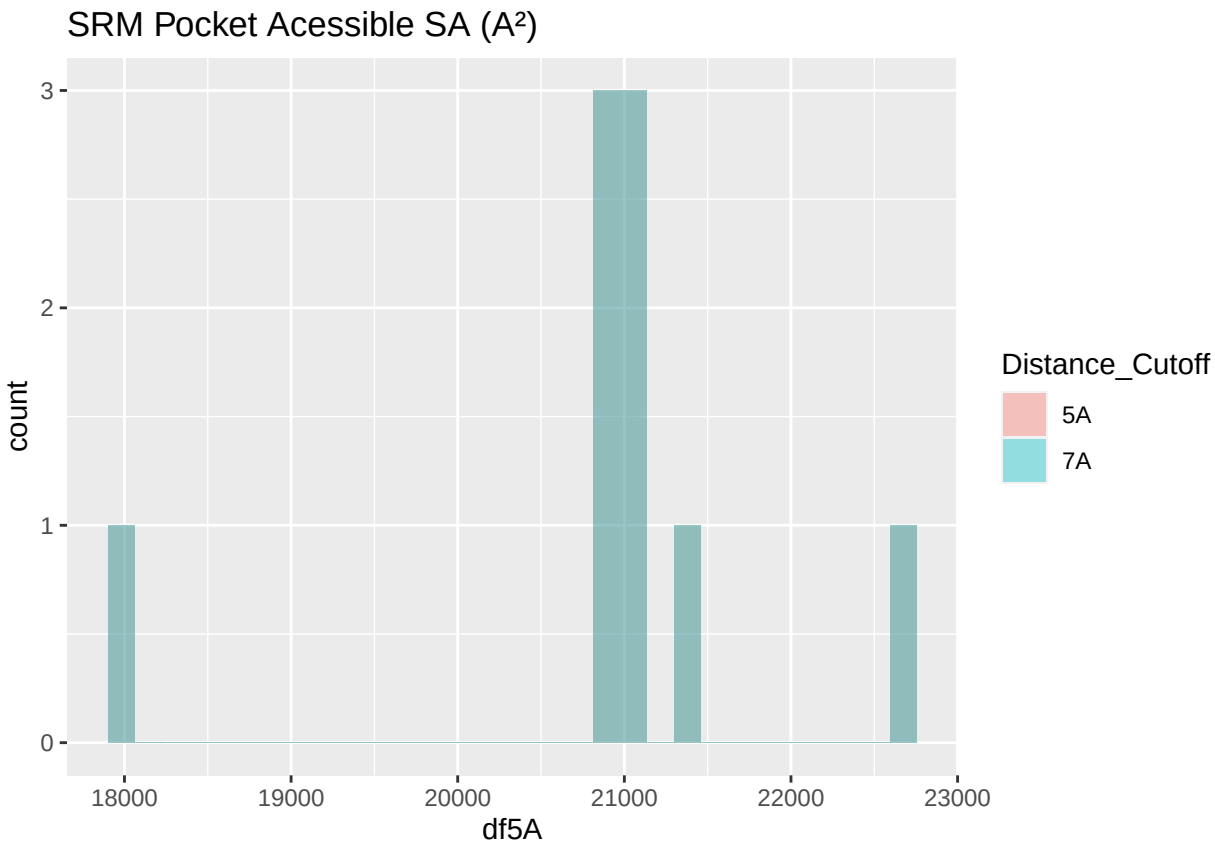

Figure 2.23: SRM: Pocket Accessible Surface Area

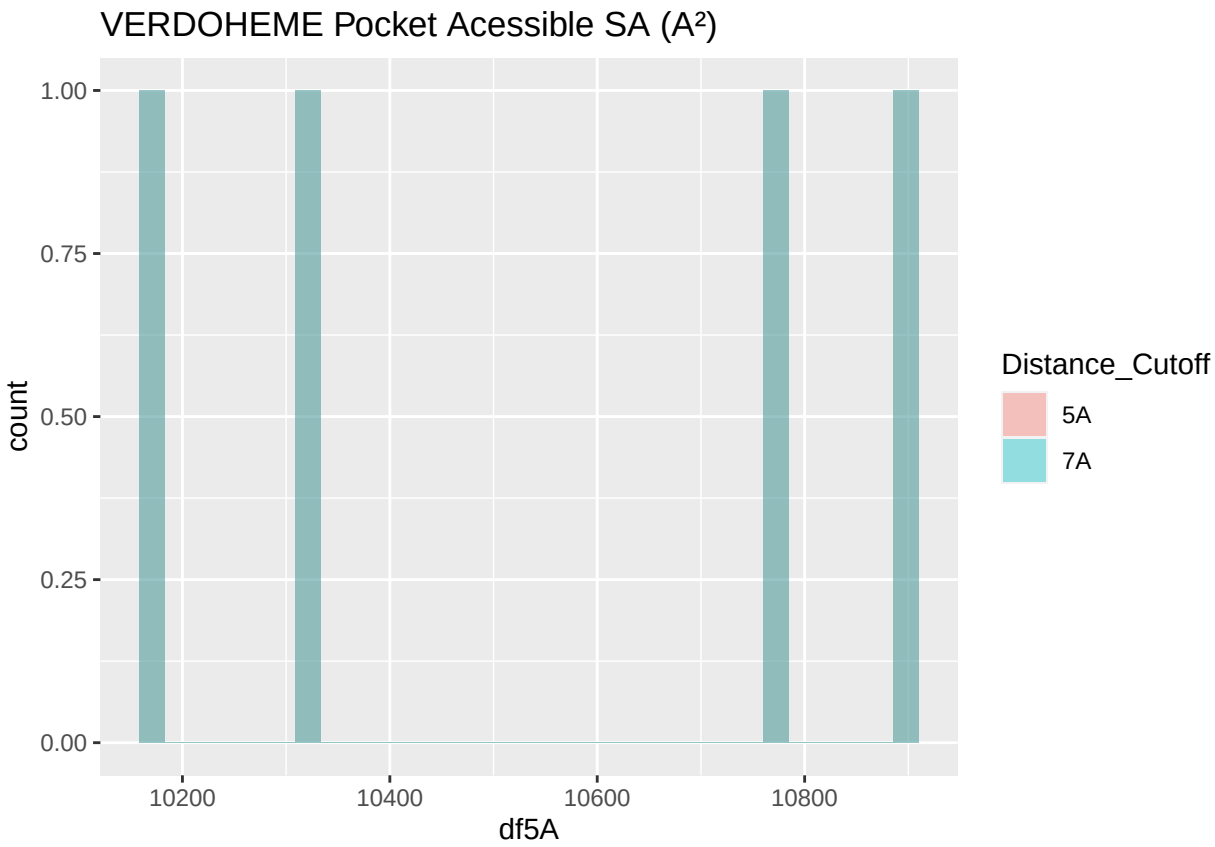

Figure 2.24: VERDOHEME: Pocket Accessible Surface Area

The surface area of binding pockets is more varied than the heme surface areas.

Heme-b and verdoheme, being highly similar molecules, with the same propionate groups, and one the derivative of the other, have quite similar surface areas, centering around 10,000-11,000 A^2. This is useful as a baseline to discuss the surface area of the binding pockets of the other two heme molecules below.

The surface area of the binding pocket of heme-c is considerably lower than that of heme-b and verdoheme. Its values center around 7500 A^2. Heme-c is bound covalently to the hemoprotein, forming thioether bonds with cysteine residues at two sites; this result suggests that the covalent bonds may exclude these sites from interacting with water molecules. Further study would be required to confirm this phenomenon.

The surface area of siroheme's binding pocket is far greater than that for other heme molecules: values center around 21000 A^2. Siroheme's extra groups on the

porphyrin ring do not appear to affect its own surface area, per above. However, it is effectively a very polar molecule and appropriately the binding pocket is highly saturated with very polar amino acids, as seen in the amino acid frequency analysis. The binding pocket is therefore completely different from the other heme molecules, and these populous, polar amino acids favorably interact with aqueous solvent, negating the need to bury any hydrophobic residues and reduce surface area.

2.6 Angular Data

As briefly mentioned in the introduction, angular data was generated but will not be discussed extensively. Figures may be found in Appendix A.4 and A.5 data tables may be found in Appendix B.5 and B.6. Amongst the results are tight distributions of planar angles and CA-CB-Fe angles for some residues; but much of the data demonstrates a broad range of angles that may be formed. The data may be useful for protein engineering and residue placement, but cannot be productively discussed and are therefore relegated to the appendices.

2.7 Limitations of the Study

A high throughput framework was built to conduct this study. However, guaranteeing the quality of PDBs to enable the scripts to function properly proved challenging, and the sample size is small, although diverse. This problem only exists for heme-b and heme-c – for siroheme and verdoheme, all structures in the PDB capable of being used, were used. Heme-b and heme-c would only require more trial and error, or pre-processing, to be input to the framework that has been built.

Although many hypotheses have been suggested in the discussion to explain the data, limited experimental data exists to confirm them. Future work may include wet lab experiments to confirm these hypotheses, such as mutating several hemoproteins to contain higher or lower percentages of nonpolar residues in the binding pocket, and observing how the binding of heme is affected.

Some of these data could also be analyzed more thoroughly, for example eliminating the coordinating amino acids from the amino acid frequency data. This was not possible here due to how the framework is constructed: coordinating residues are not identified, nor is a definition proposed to identify coordinating residues. Manual input of known coordinating residues would be necessary to be certain that they could be eliminated from the final dataset analyzed, but this was beyond the scope of this study.

UCSF-Chimera was used to generate all data used in this study; many algorithms have remained unchanged for some time (surface area calculations are sourced from MSMS (1996) and volume calculations from Surfnet (1995)). It would be well to compare with any new algorithms that are developed to calculate surface area or volume, or with any experimental data that may be used confirm these numbers.

The reason being for this desired orthogonality is that the algorithms themselves may certainly introduce bias based off how they work. Surfnet generates 3D-contour surfaces to identify cavities; in practice, many small "bubbles" or insignificant cavities were generated in the study, and are filtered out during analysis – the parameters chosen can also significantly influence the behavior of the algorithm; in this study, the default parameters appeared to generate the most reasonable binding pocket. But this assessment is based off subjective visual observation by the author, and therefore introduces further bias. One may expect applying the same algorithm with the same parameters to many PDBs may at least introduce the same bias to all samples, but the algorithm may distort some PDBs more than others depending on the shape and size of their binding pocket.

3
Conclusion

A knowledge gap in the binding environment for heme exists in the present literature. A high-throughput framework employing UCSF Chimera was constructed to process diverse sets of hemoproteins and output information about their binding pockets: amino acid frequencies and distances from heme, volume, surface area, angles. Data was gathered and predicted from representative and varied datasets for heme-b, heme-c, verdoheme, and siroheme, and their respective hemoproteins. R was used to analyze all data.

The results of this study suggest that binding pockets for hemoproteins have some requirements for binding that may have been overlooked to date. The data and their trends observed in this study demonstrate several phenomena.

First, the heme binding environments for heme-b, heme-c, and verdoheme contain high populations of nonpolar amino acids, suggesting nonpolar interactions may be of greater importance than previously thought to providing the necessary interactions to bind heme. The binding environment for siroheme, by contrast, is shown to be extremely enriched with polar amino acids, which is not very surprising; but this binding environment also still contains many nonpolar amino acids, reinforcing the idea that the polar interactions for all heme molecules, while necessary, may be insufficient for heme binding.

Second, most of the volume data for the binding pockets of all heme molecules centers around a value of 1200 A^3. Surface areas of heme-b and verdoheme binding pockets are similar, approximately 10000 A^2, the surface area for heme-c is less, approximately 7500 A^2, and for siroheme is approximately 21000 A^2. These values may be useful in the design of artifical metalloenzymes.

Additionally, the seeming conservation of the volume size but the variety in pocket surface areas demonstrates that while the heme molecules may be of similar size and, besides attached groups, similar structure, the attached groups will significantly affect what interactions occur in the binding pockets, and therefore the shape and exposure to solvent in the binding pockets. Siroheme is strongly polar and its binding pocket has a large surface area and is therefore highly solvent exposed, as compared to heme-b which has more nonpolar groups that must be buried and therefore requiring a smaller surface area.

Finally, angular data were generated; but the phenomena observed, such as some residues having tight ranges of angles in relation to heme or the heme iron, cannot be interpreted as useful results, except perhaps for some protein engineering efforts that may have interest in the range or distribution of possible angles for a specific residue.

These results may be useful for the rational design of hemoproteins, with the importance of nonpolar interactions in particular likely of great interest. The framework constructed for this study can be applied to any list of PDBs and their respective ligands, thereby facilitating similar research for other proteins.

Appendices

A
Figures

A.1 AA Frequency

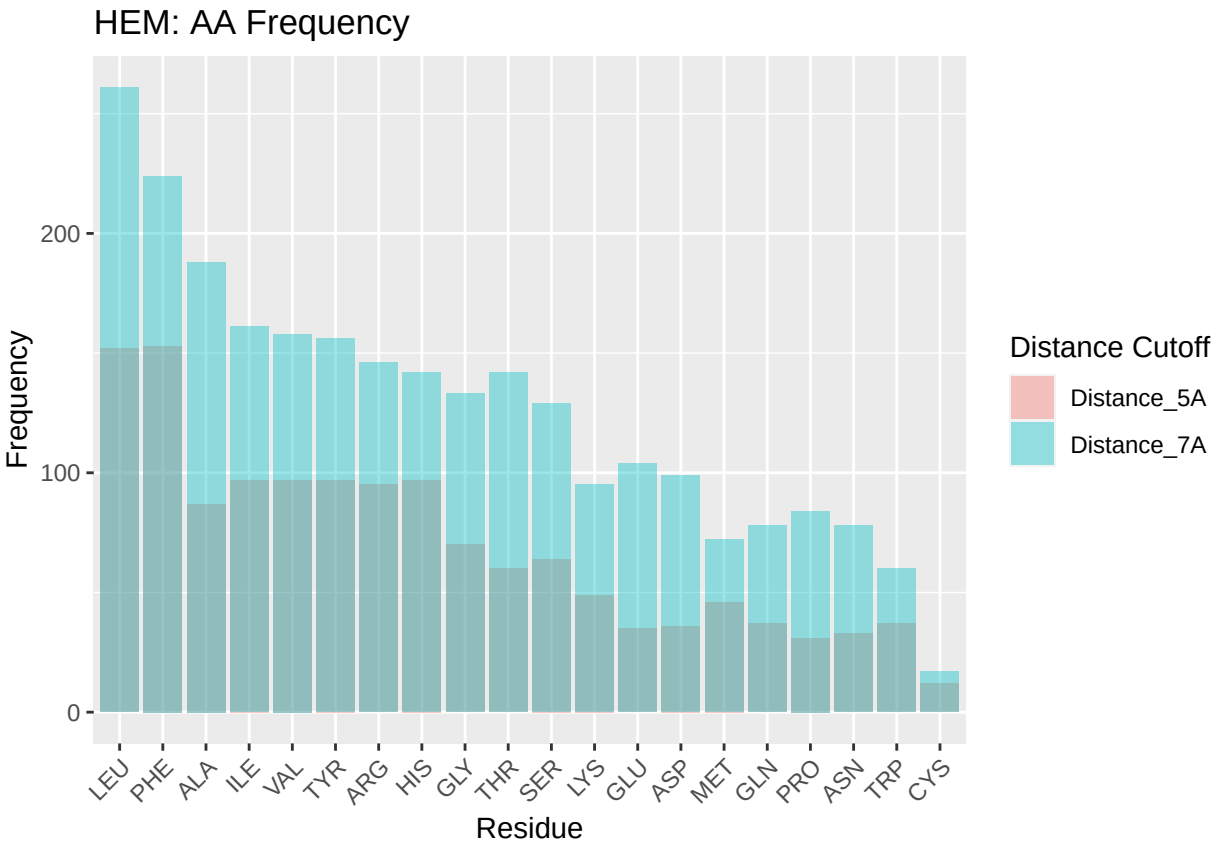

Figure A.1: HEM: AA Frequency

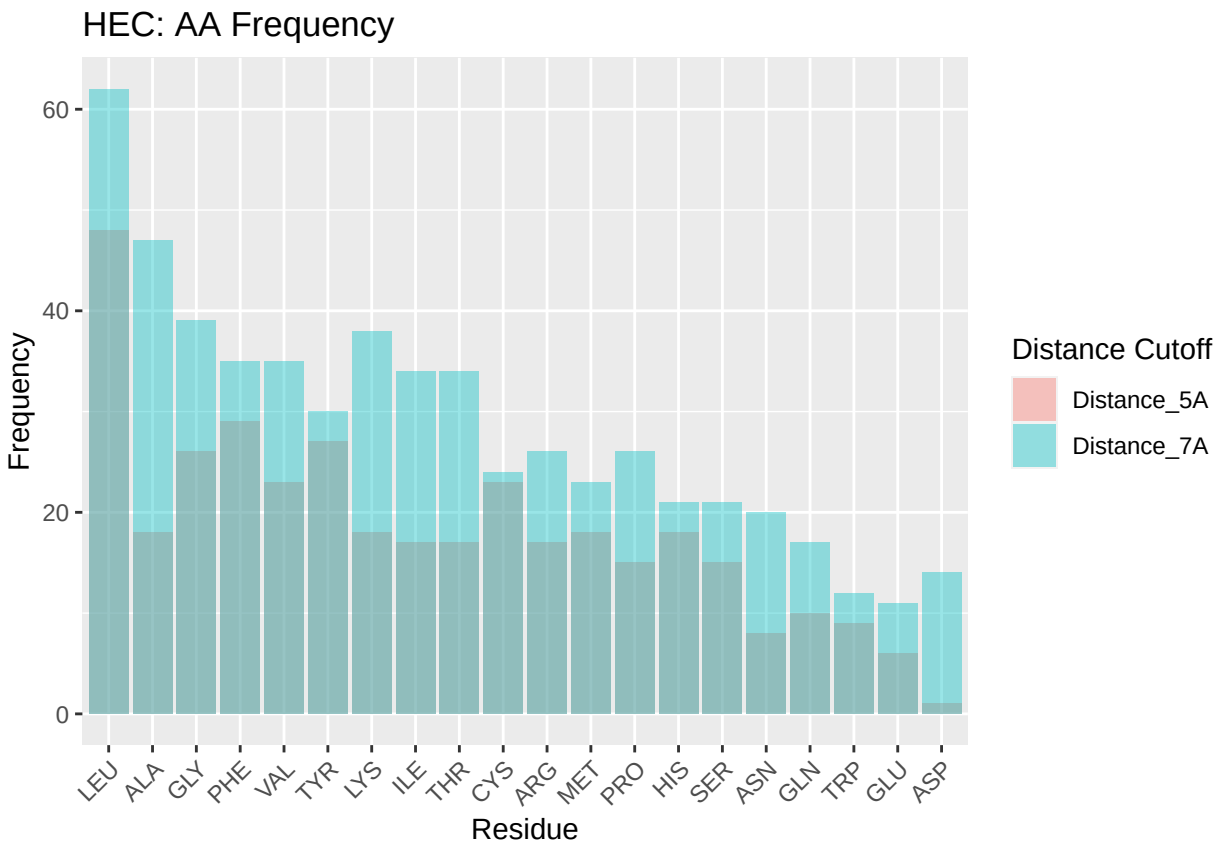

Figure A.2: HEC: AA Frequency

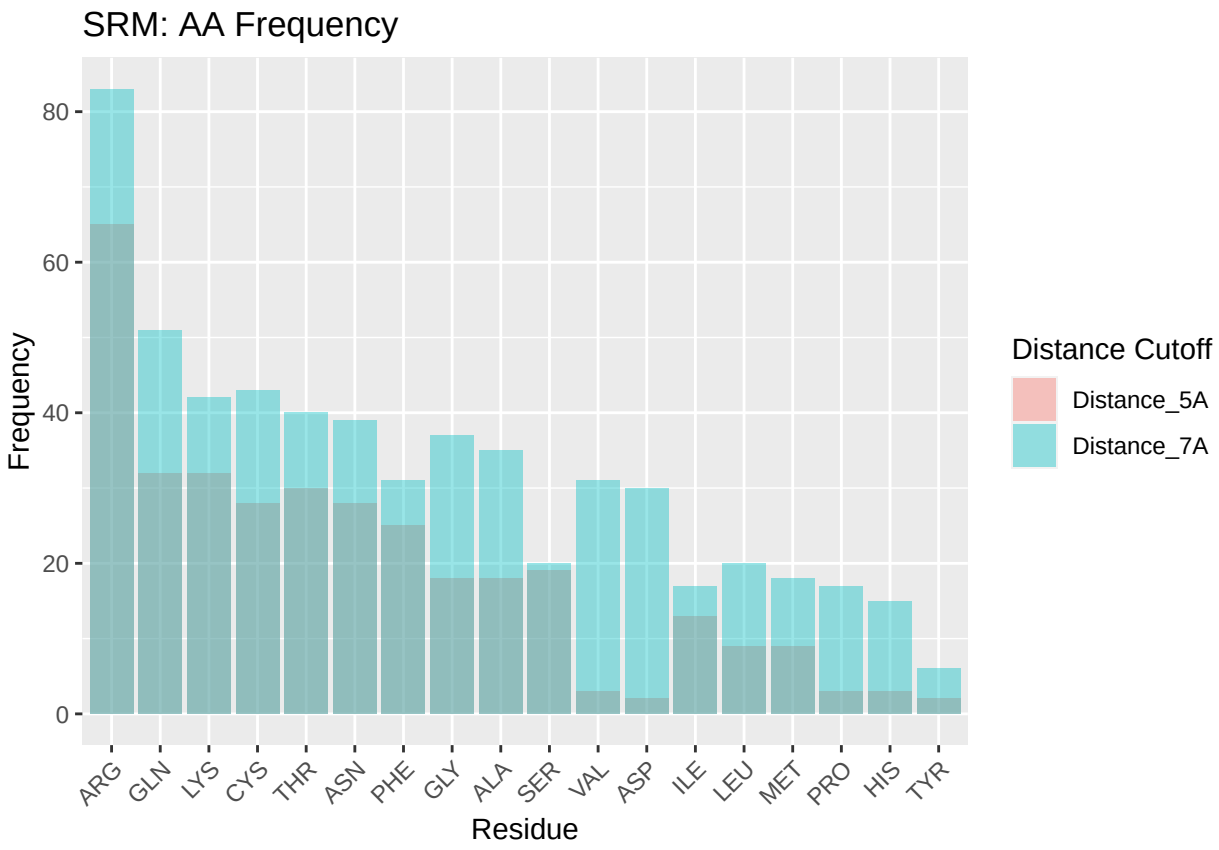

Figure A.3: SRM: AA Frequency

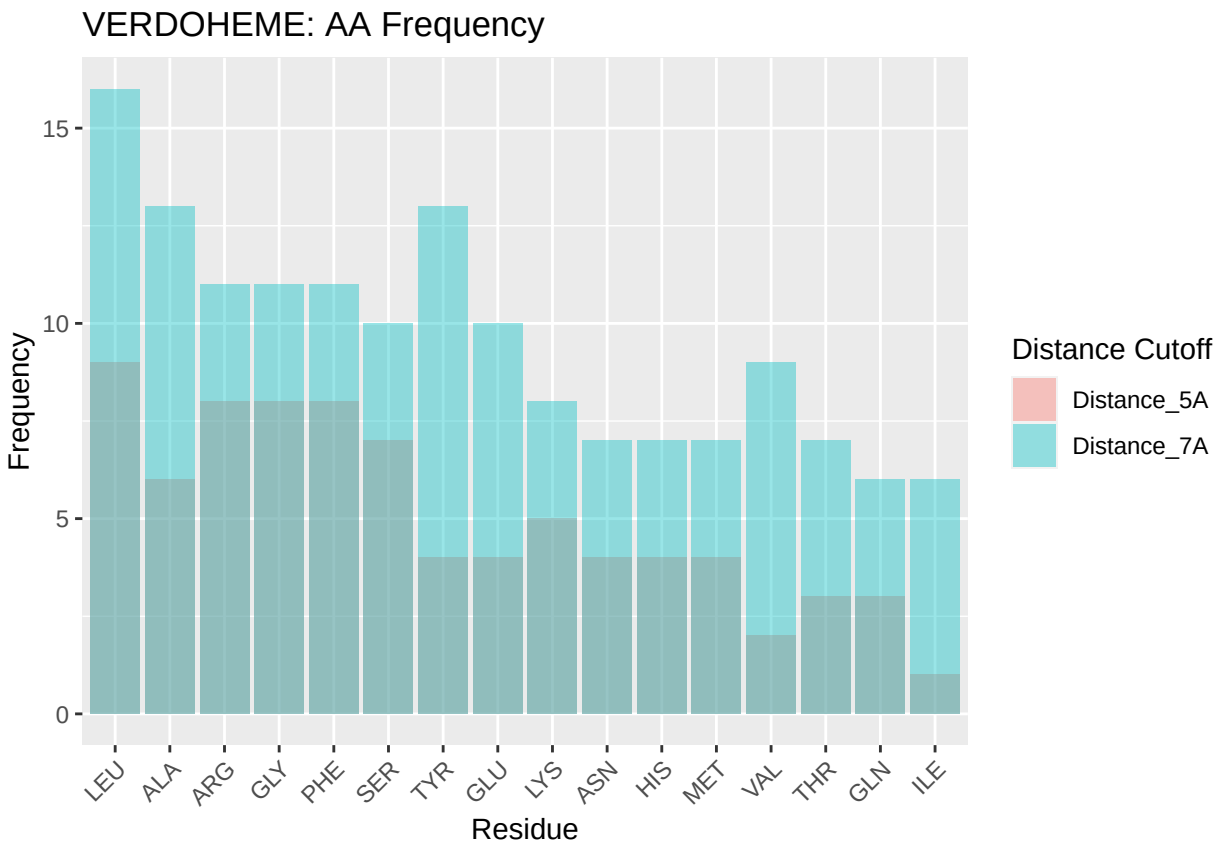

Figure A.4: VERDOHEME: AA Frequency

A.2 Ligand Excluded Surface Area

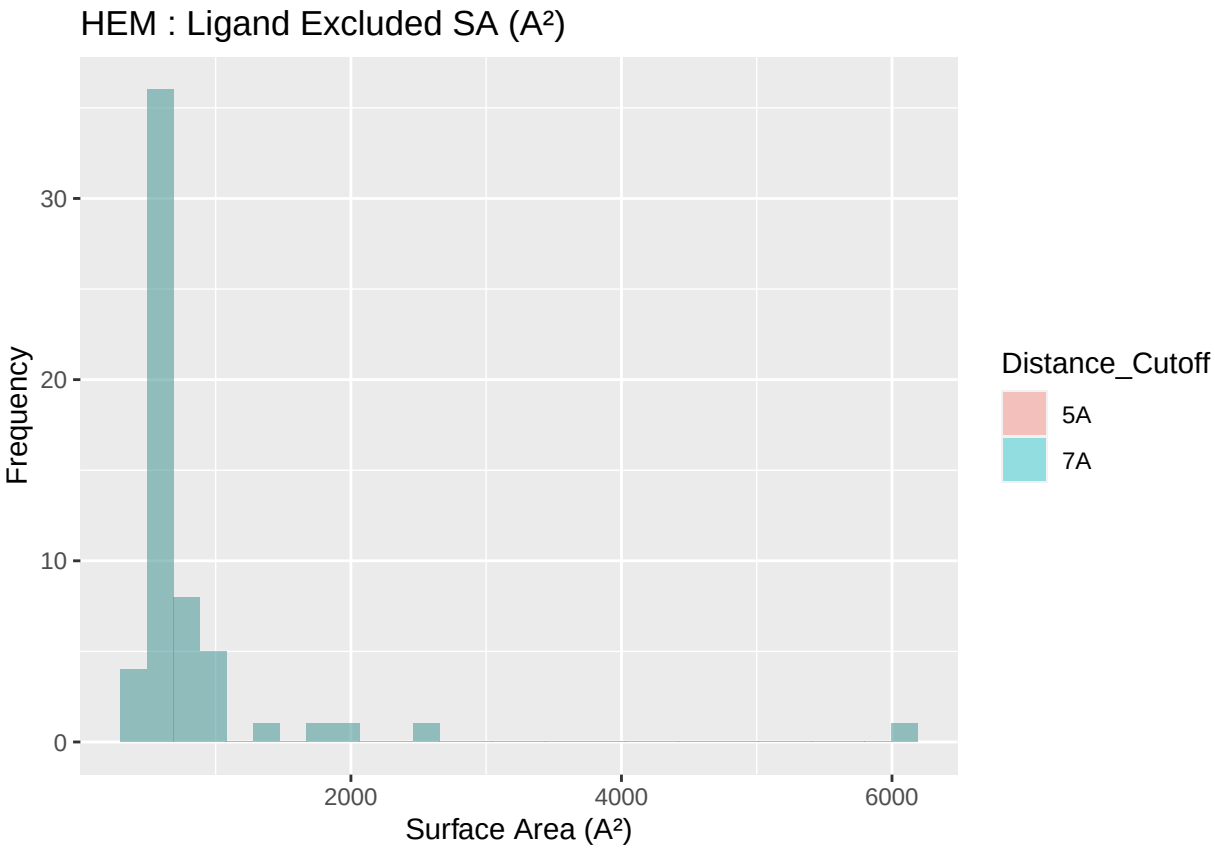

Figure A.5: HEM: Ligand Excluded Suface Area

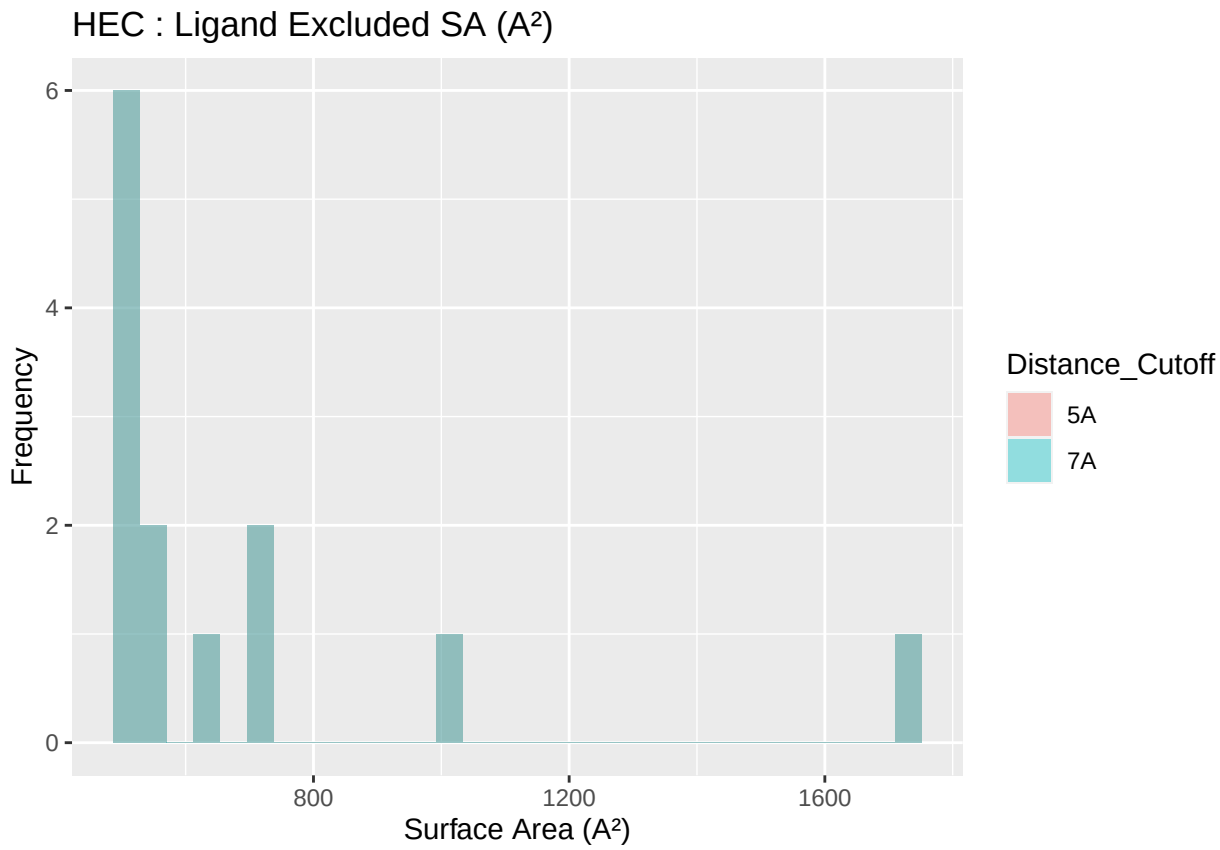

Figure A.6: HEC: Ligand Excluded Suface Area

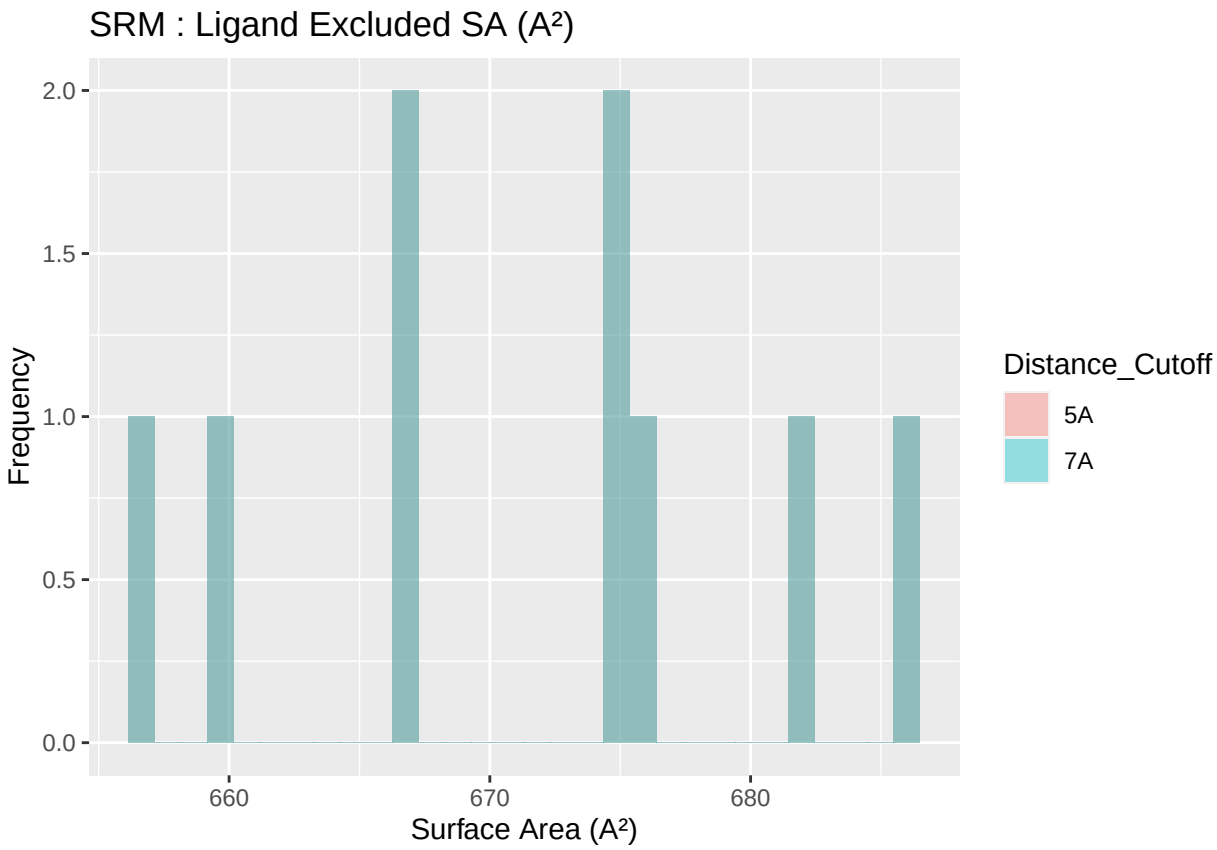

Figure A.7: SRM: Ligand Excluded Suface Area

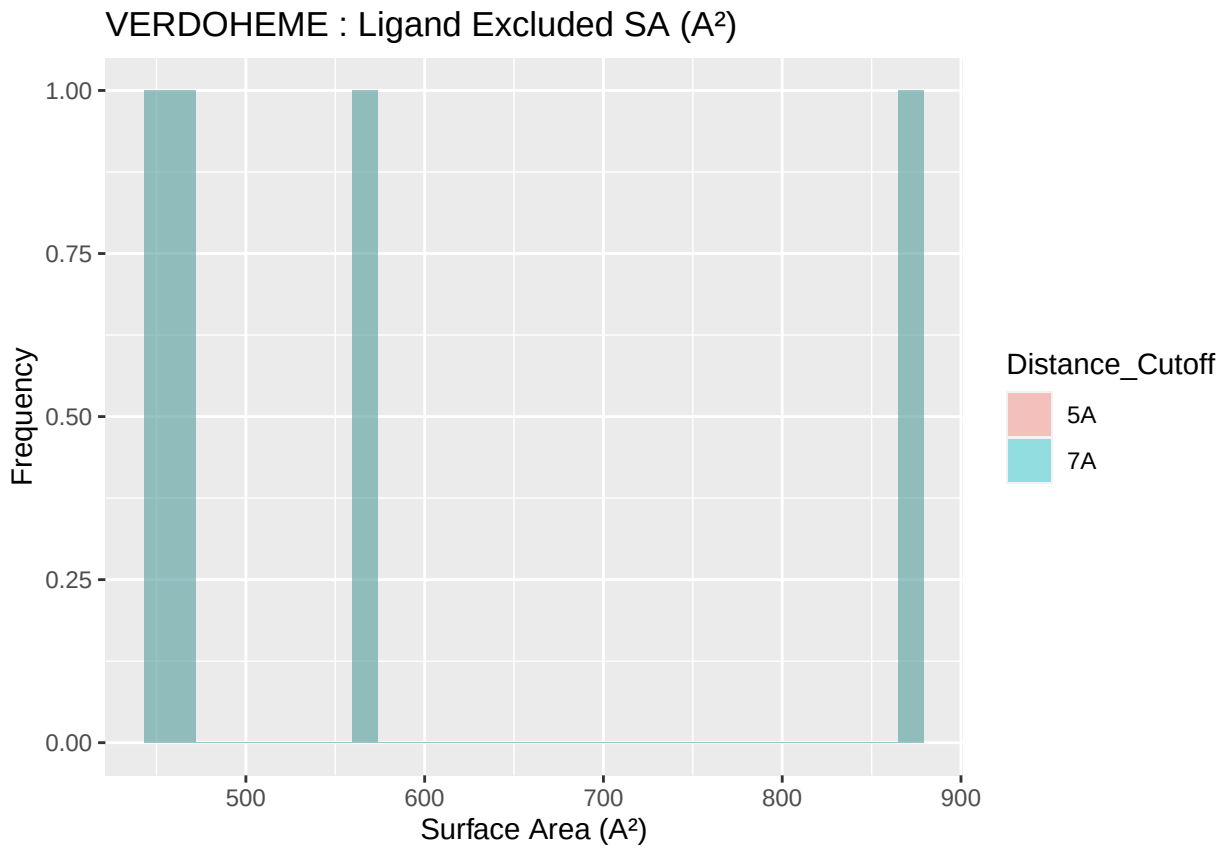

Figure A.8: VERDOHEME: Ligand Excluded Suface Area

A.3 Pocket Excluded Surface Area

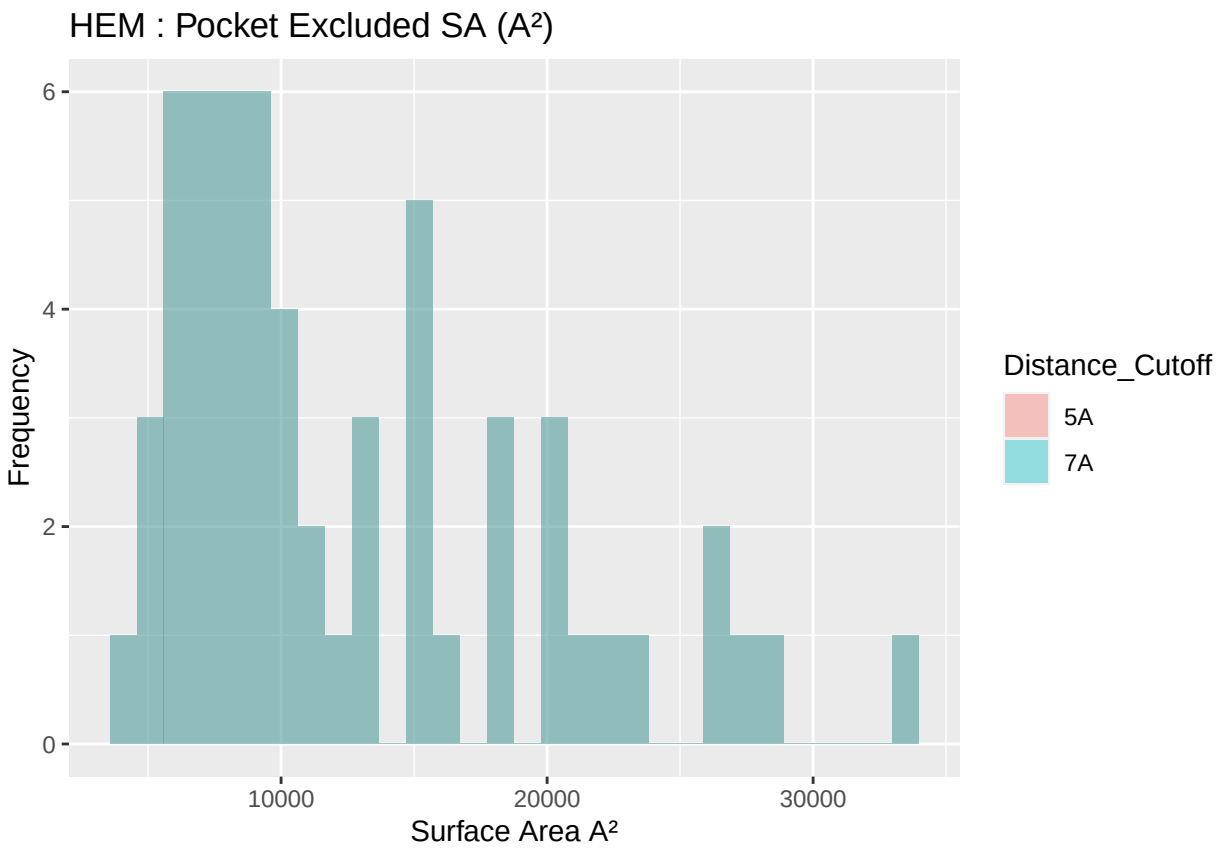

Figure A.9: HEM: Pocket Excluded Surface Area

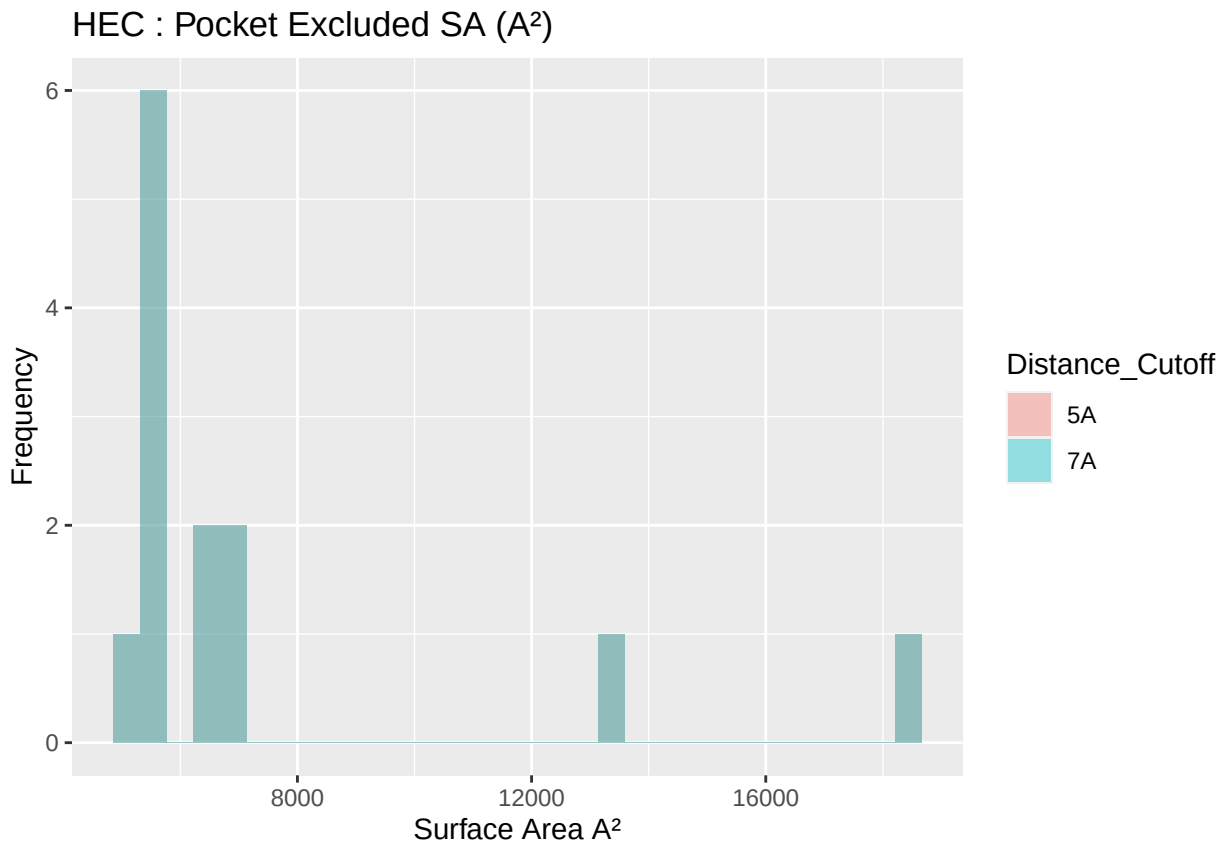

Figure A.10: HEC: Pocket Excluded Surface Area

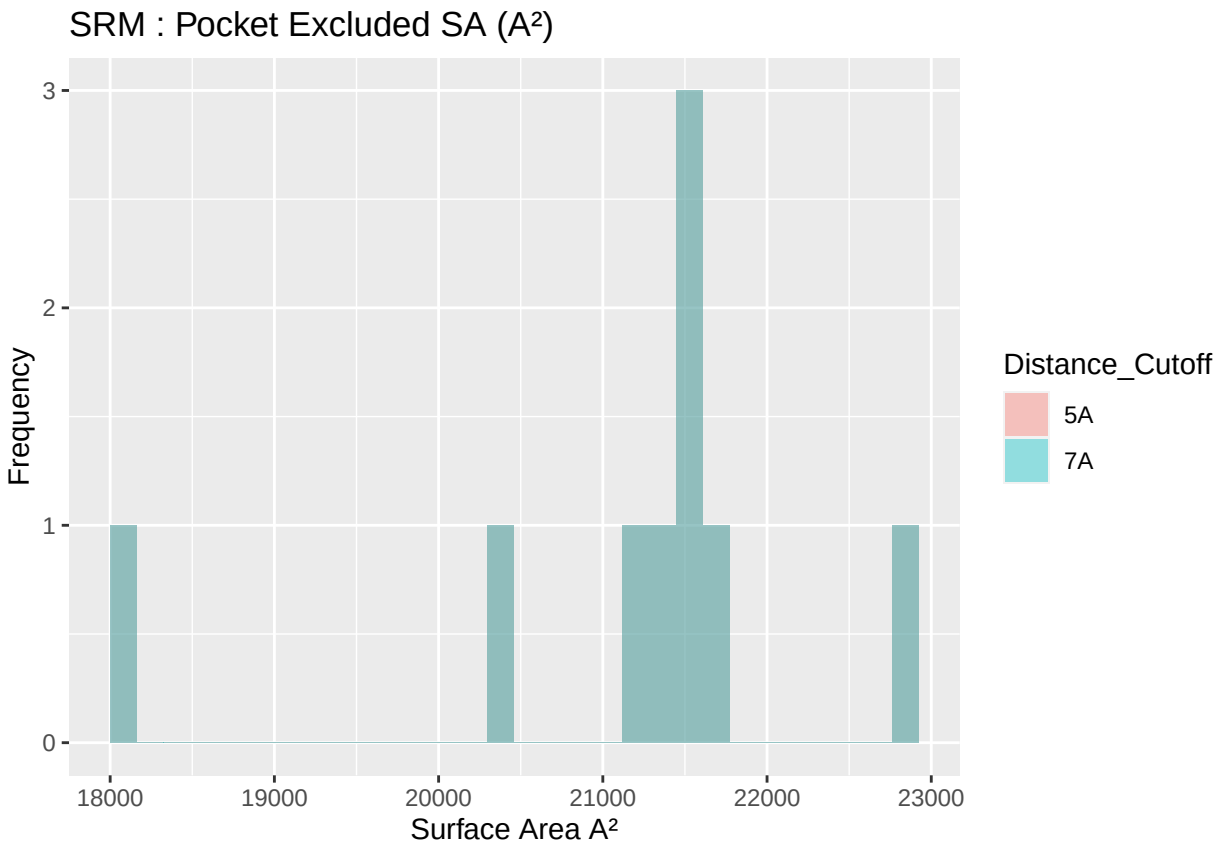

Figure A.11: SRM: Pocket Excluded Surface Area

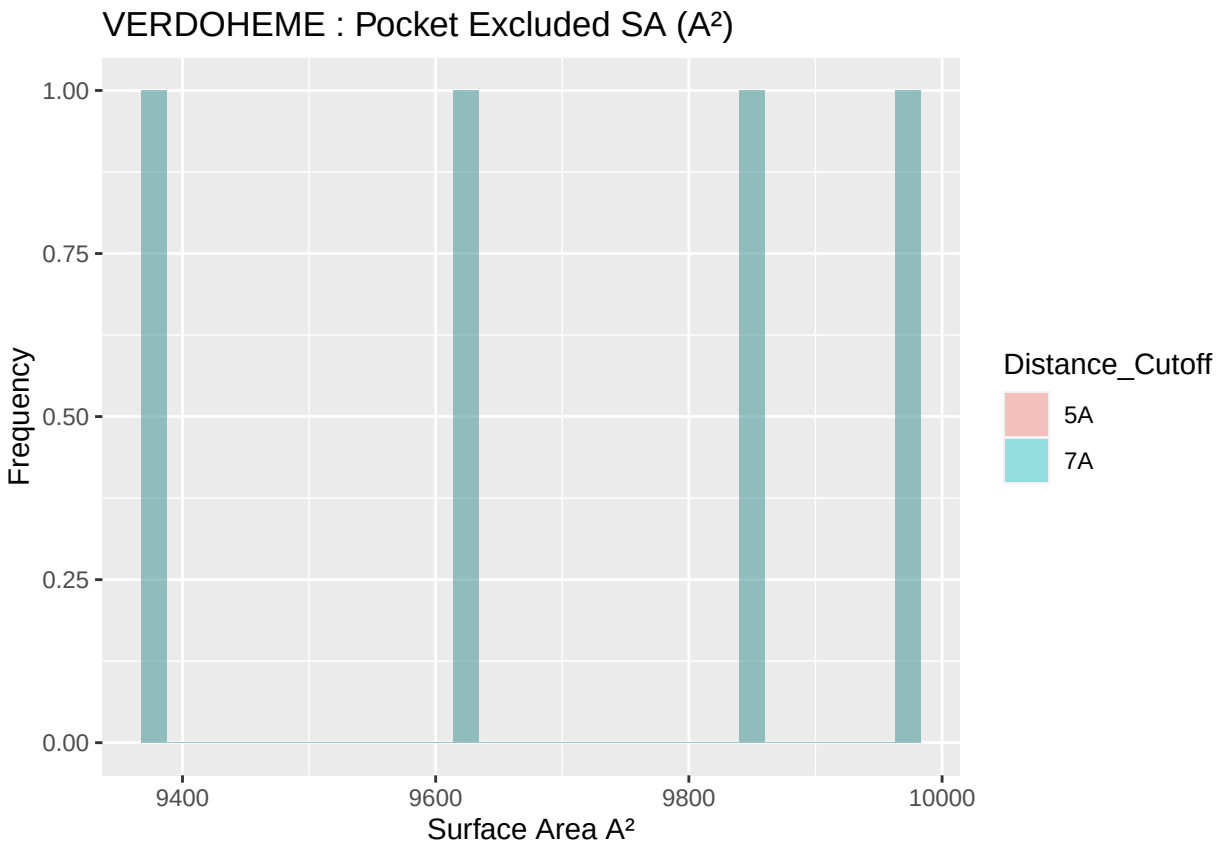

Figure A.12: VERDOHEME: Pocket Excluded Surface Area

A.4 All Planar Angles

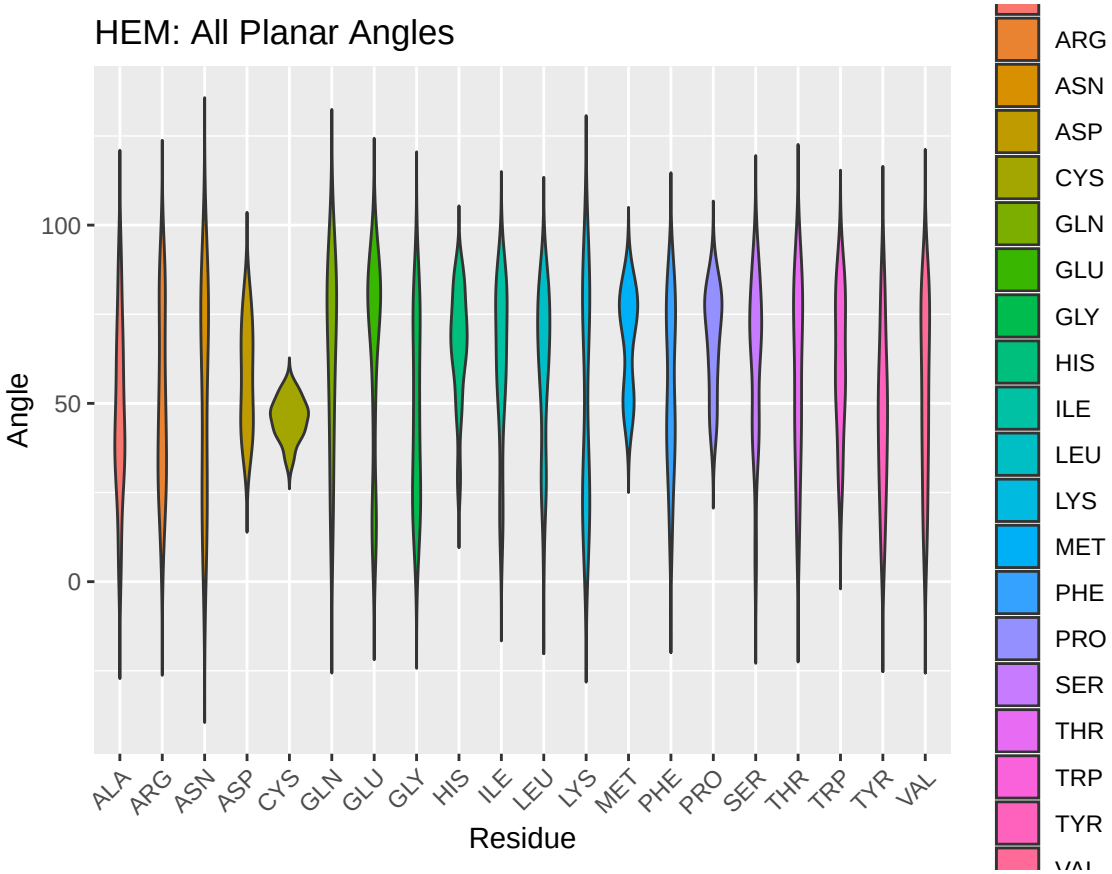

Figure A.13: HEM: All Planar Angles

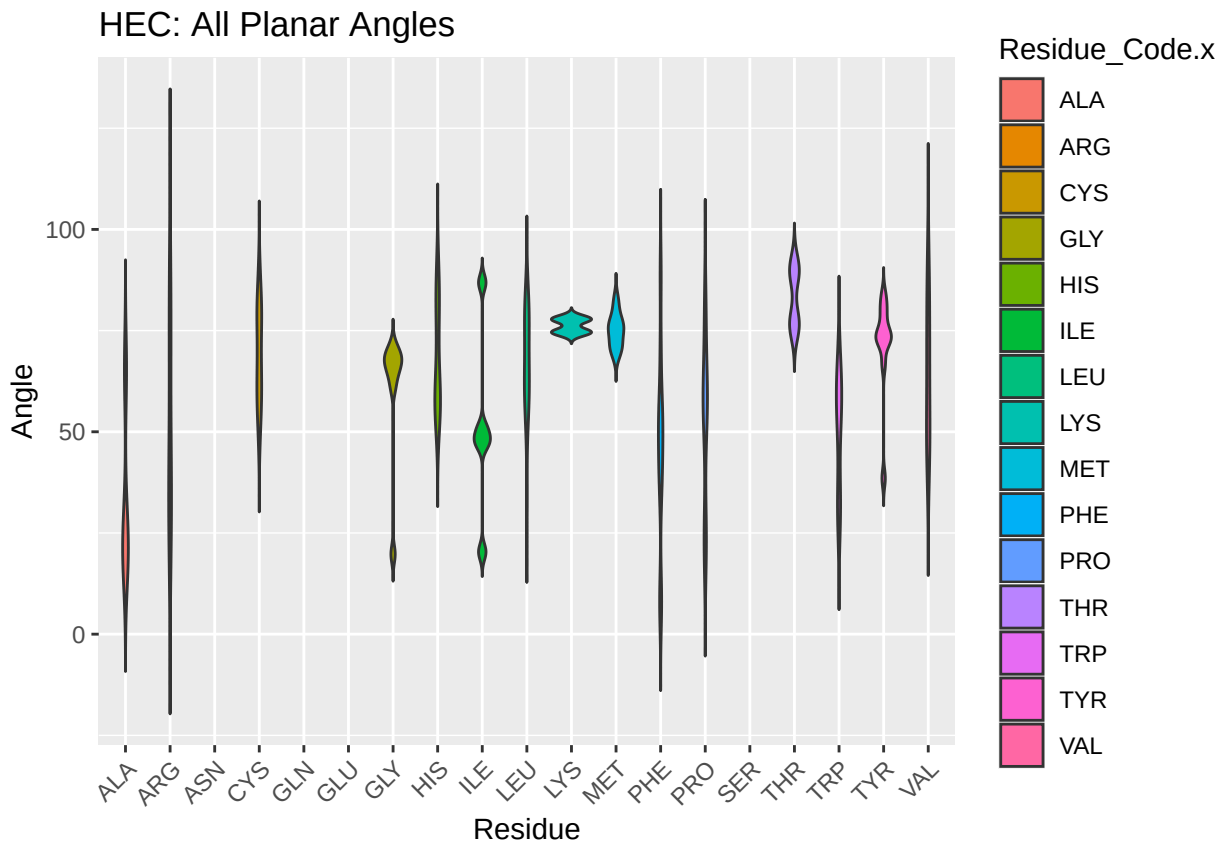

Figure A.14: HEC: All Planar Angles

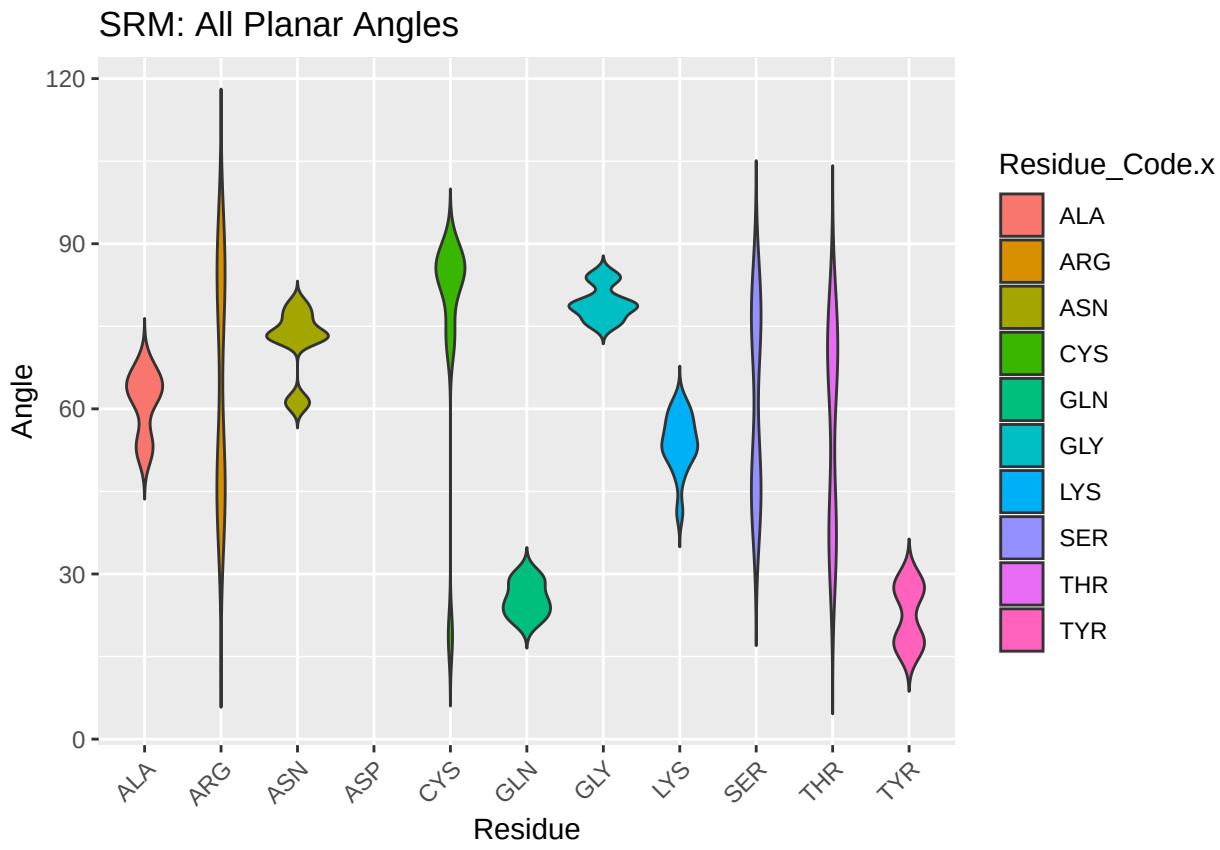

Figure A.15: SRM: All Planar Angles

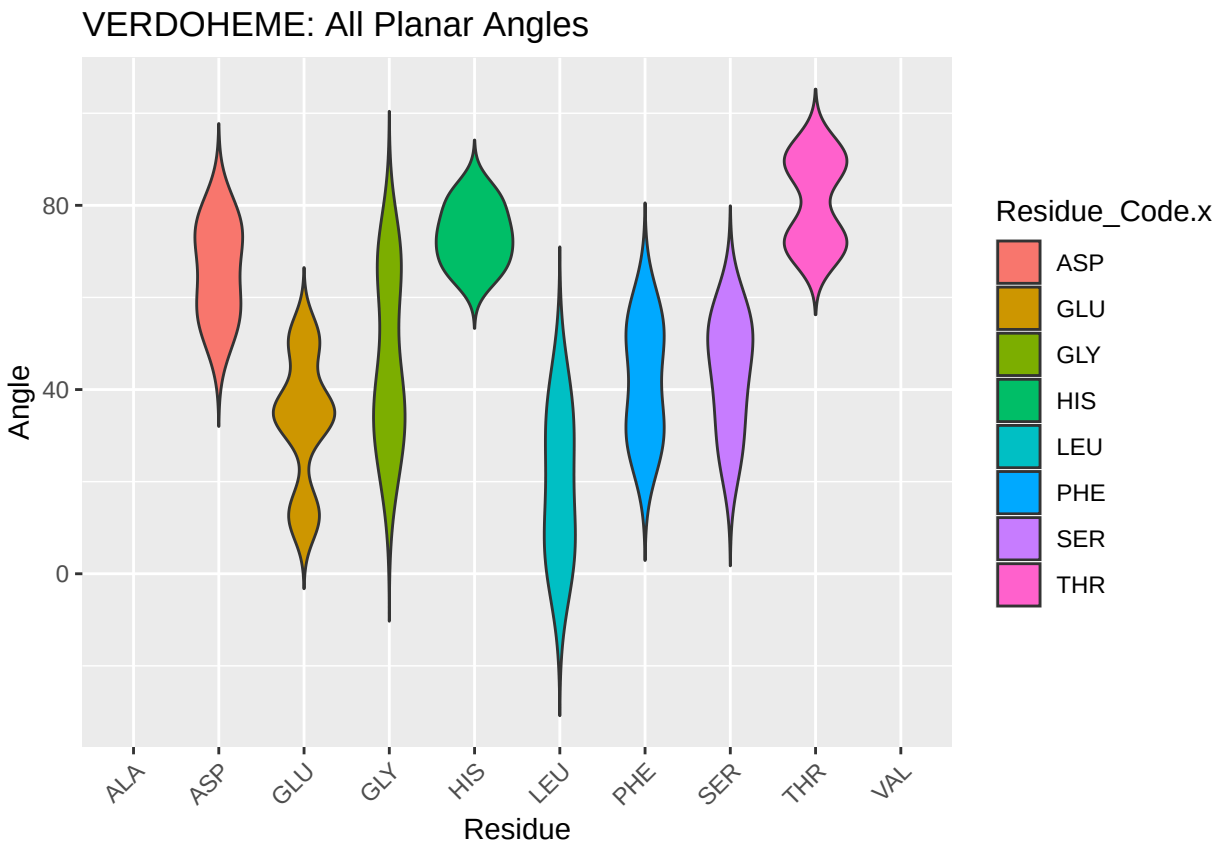

Figure A.16: VERDOHEME: All Planar Angles

A.5 All CA-CB-Fe Angles

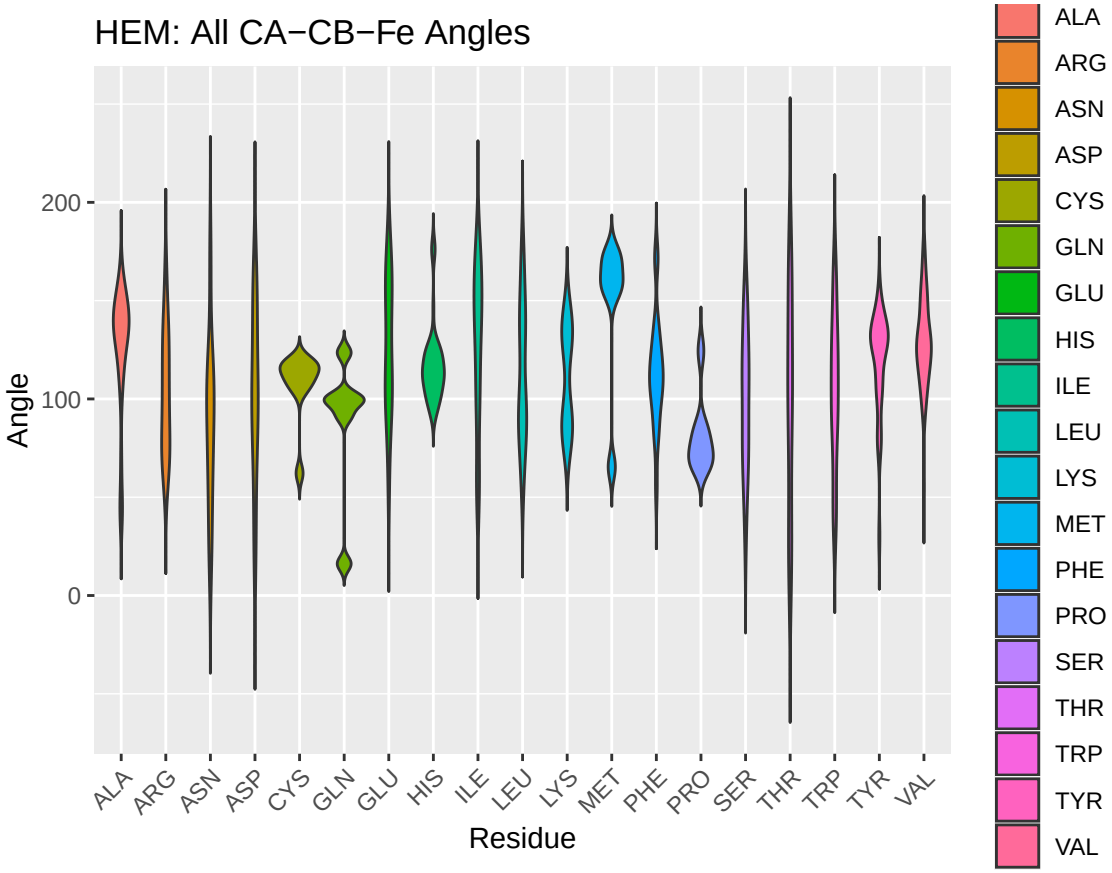

Figure A.17: HEM: All CA-CB-Fe Angles

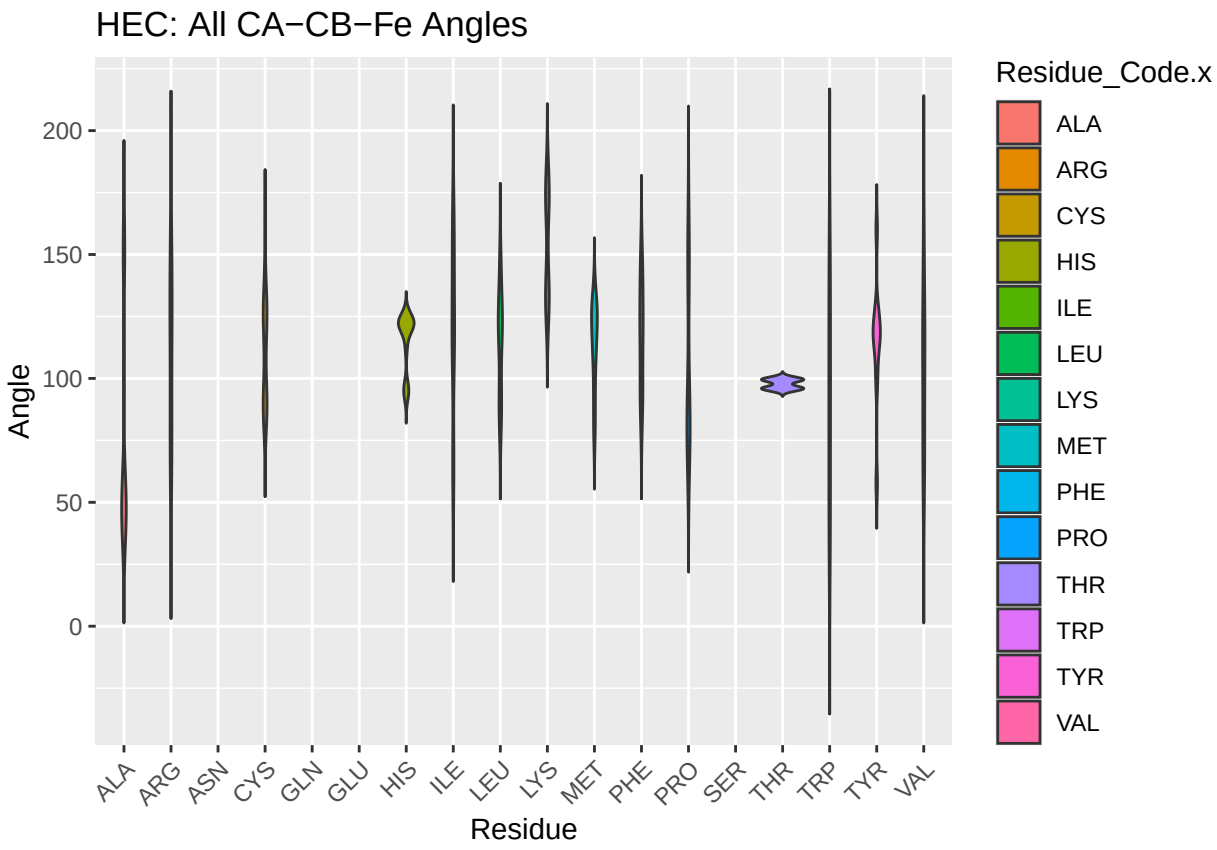

Figure A.18: HEC: All CA-CB-Fe Angles

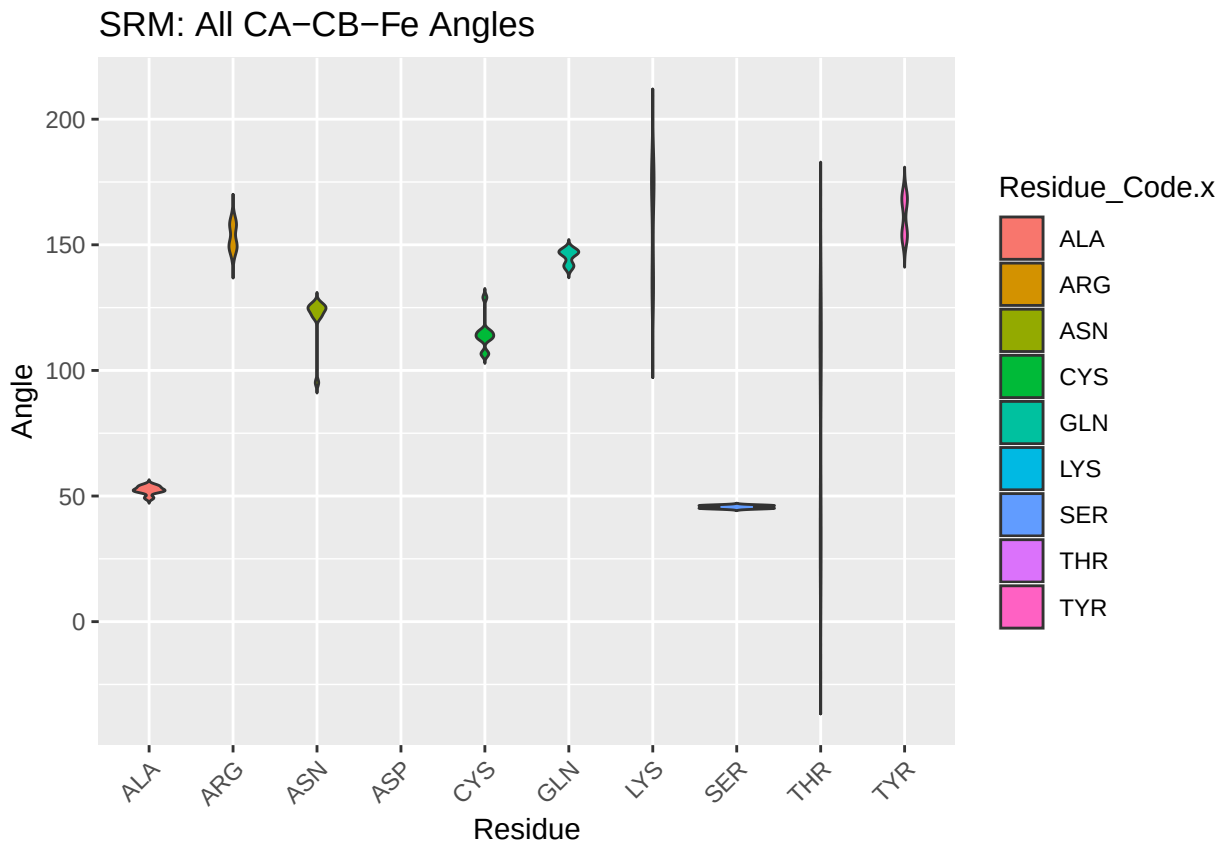

Figure A.19: SRM: All CA-CB-Fe Angles

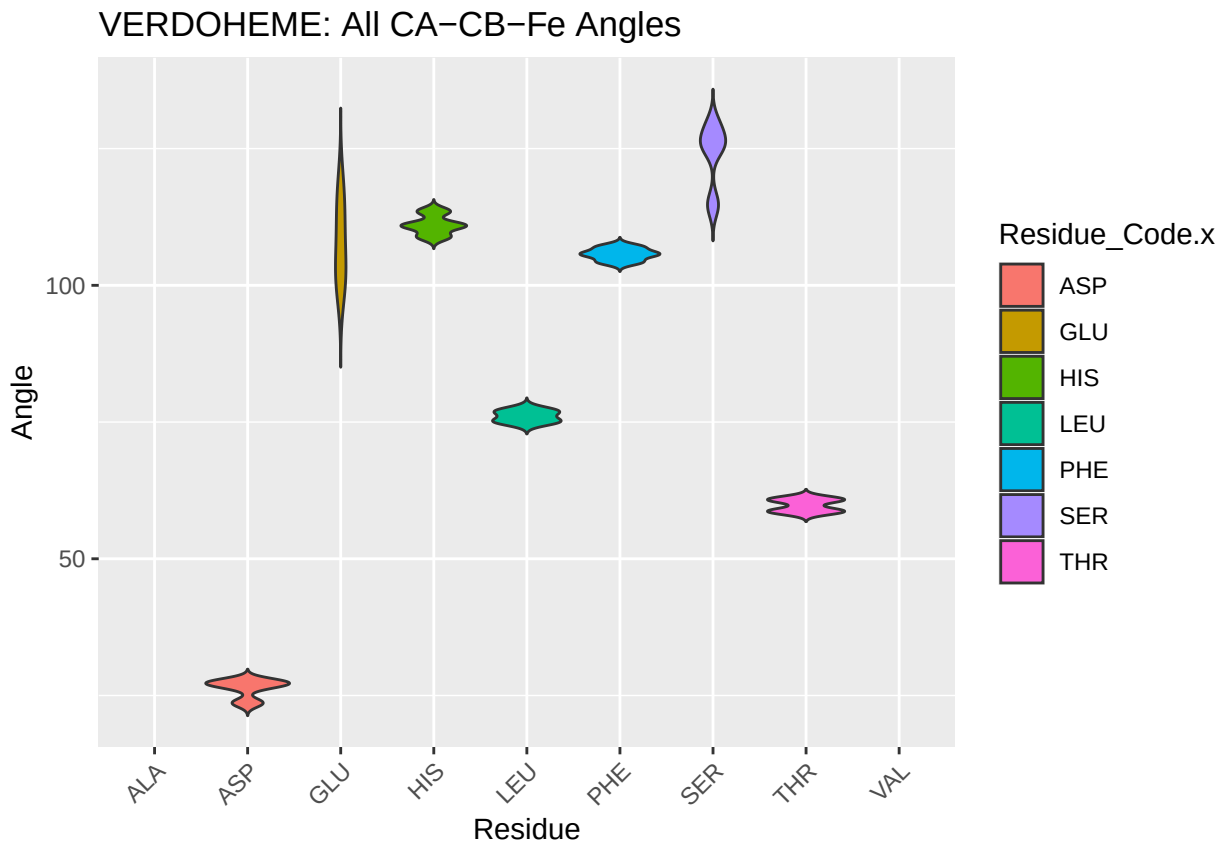

Figure A.20: VERDOHEME: All CA-CB-Fe Angles

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;
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 Amino Acid Frequencies at 5A Distance Cutoff

Table B.5: HEM AA Freq, Cutoff 5A

Residue	Freq
PHE	153
LEU	152
HIS	97
ILE	97
TYR	97
VAL	97
ARG	95
ALA	87
GLY	70
SER	64
THR	60
LYS	49
MET	46
GLN	37
TRP	37
ASP	36
GLU	35
ASN	33
PRO	31
CYS	12

Table B.6: HEC AA Freq

Residue	Freq
LEU	48
PHE	29
TYR	27
GLY	26
CYS	23
VAL	23
ALA	18
HIS	18
LYS	18
MET	18

Table B.6: HEC AA Freq *(continued)*

Residue	Freq
ARG	17
ILE	17
THR	17
PRO	15
SER	15
GLN	10
TRP	9
ASN	8
GLU	6
ASP	1

Table B.7: VERDOHEME AA Freq

Residue	Freq
LEU	9
ARG	8
GLY	8
PHE	8
SER	7
ALA	6
LYS	5
ASN	4
GLU	4
HIS	4
MET	4
TYR	4
GLN	3
THR	3
VAL	2
ILE	1

Table B.8: SRM AA Freq

Residue	Freq
ARG	65
GLN	32
LYS	32
THR	30

Table B.8: SRM AA Freq *(continued)*

Residue	Freq
ASN	28
CYS	28
PHE	25
SER	19
ALA	18
GLY	18
ILE	13
LEU	9
MET	9
HIS	3
PRO	3
VAL	3
ASP	2
TYR	2

B.3 Distances

B.3.1 All Distances from Heme Fe to Atoms of Residues in Binding Pocket

Table B.9: HEM: All Distances, Atoms to Fe

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1	1B2V	HIS	83	ND1	4.091840
2	1B2V	TYR	75	CG	5.370524
3	1B2V	VAL	37	CG2	5.119564
4	1B2V	HIS	83	NE2	5.795310
5	1B2V	VAL	37	CG1	5.302293
6	1B2V	LEU	77	CA	6.357591
7	1B2V	SER	42	O	6.611193
8	1B2V	HIS	83	CA	5.317261
9	1B2V	LEU	77	N	6.764107
10	1B2V	TYR	75	CZ	2.888333
11	1B2V	TYR	75	CE1	3.676968

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
12	1B2V	TYR	75	CD2	4.821397
13	1B2V	TYR	75	CD1	4.880663
14	1B2V	TYR	75	CB	6.798699
15	1B2V	TYR	75	CE2	3.624167
16	1B2V	HIS	83	CE1	4.910880
17	1B2V	HIS	32	CE1	3.237980
18	1B2V	HIS	32	CD2	3.186876
19	1B2V	HIS	32	ND1	4.330731
20	1B2V	HIS	32	CB	5.756445
21	1B2V	HIS	32	O	5.953564
22	1B2V	HIS	32	C	6.358164
23	1B2V	MET	140	CE	5.777781
24	1B2V	MET	140	SD	6.659910
25	1B2V	HIS	83	CB	4.758791
26	1B2V	HIS	32	CA	6.565816
27	1B2V	TYR	75	OH	1.954327
28	1B2V	SER	42	OG	5.900798
29	1B2V	SER	42	CB	6.636304
30	1B2V	HIS	32	CG	4.355931
31	1B2V	LEU	77	O	6.769296
32	1B2V	TYR	137	CE1	6.096698
33	1B2V	SER	42	CA	6.625250
34	1B2V	TYR	137	CD1	6.368337
35	1B2V	HIS	83	CG	4.725560
36	1B2V	HIS	83	O	5.883823
37	1B2V	HIS	83	C	5.884565
38	1B2V	ASN	41	O	6.894251
39	1B2V	HIS	83	N	6.545924
40	1B2V	VAL	37	CB	5.853806
41	1B2V	THR	84	N	6.798527
42	1B2V	HIS	83	CD2	5.752036
43	1B2V	HIS	32	NE2	2.263051
44	1B2V	LEU	77	CD1	5.828324
45	1B5M	HIS	63	NE2	1.819890
46	1B5M	HIS	63	CE1	3.023255

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
47	1B5M	HIS	63	CD2	2.588060
48	1B5M	HIS	63	ND1	4.027399
49	1B5M	HIS	63	CG	3.837789
50	1B5M	HIS	63	CB	5.198178
51	1B5M	PRO	40	CD	5.362624
52	1B5M	PHE	35	CZ	5.731102
53	1B5M	HIS	63	CA	6.222160
54	1B5M	HIS	63	N	6.979191
55	1B5M	GLY	62	O	6.365897
56	1B5M	PRO	40	CG	6.038149
57	1B5M	VAL	61	CG2	6.762820
58	1B5M	VAL	61	CG1	5.208622
59	1B5M	VAL	61	CB	6.253291
60	1B5M	PRO	40	CB	6.380659
61	1B5M	HIS	39	NE2	1.918499
62	1B5M	LEU	46	CD2	5.100407
63	1B5M	LEU	46	CD1	6.238688
64	1B5M	LEU	46	CG	6.207115
65	1B5M	PRO	40	C	6.098869
66	1B5M	VAL	45	CG1	5.846522
67	1B5M	HIS	39	CG	4.056245
68	1B5M	PRO	40	CA	6.434682
69	1B5M	PHE	58	CZ	6.351848
70	1B5M	PHE	58	CE2	5.187940
71	1B5M	PHE	58	CD2	5.070064
72	1B5M	PRO	40	N	5.880309
73	1B5M	PHE	58	CG	6.133869
74	1B5M	PHE	58	CB	6.546370
75	1B5M	PHE	58	O	6.794383
76	1B5M	PHE	58	CA	6.591026
77	1B5M	HIS	39	CE1	2.767199
78	1B5M	GLY	42	O	6.731713
79	1B5M	GLY	41	O	5.998395
80	1B5M	GLY	41	C	5.685211
81	1B5M	GLY	41	CA	4.980319

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
82	1B5M	GLY	41	N	4.888585
83	1B5M	HIS	39	ND1	3.934694
84	1B5M	PHE	35	CE2	5.325081
85	1B5M	HIS	39	CD2	3.022098
86	1B5M	HIS	39	CB	5.471773
87	1B5M	HIS	39	O	6.809826
88	1B5M	HIS	39	C	6.158780
89	1B5M	GLY	42	N	6.336121
90	1B5M	PHE	35	CD2	6.489161
91	1B5M	ALA	67	CB	5.797296
92	1B5M	HIS	39	CA	5.972168
93	1DK0	HIS	32	CE1	3.097081
94	1DK0	TYR	75	CD1	4.870310
95	1DK0	TYR	75	CG	5.439675
96	1DK0	TYR	75	CB	6.855877
97	1DK0	HIS	32	CD2	3.087544
98	1DK0	TYR	137	CE1	6.058239
99	1DK0	MET	140	CE	5.680994
100	1DK0	HIS	32	ND1	4.178511
101	1DK0	MET	140	SD	6.690840
102	1DK0	VAL	37	CG2	5.172684
103	1DK0	VAL	37	CG1	5.226870
104	1DK0	VAL	37	CB	5.802353
105	1DK0	HIS	32	CG	4.227248
106	1DK0	HIS	32	CB	5.635484
107	1DK0	HIS	83	NE2	5.746185
108	1DK0	HIS	83	CD2	5.738879
109	1DK0	HIS	83	CG	4.688593
110	1DK0	SER	42	CB	6.491744
111	1DK0	HIS	83	O	5.767033
112	1DK0	TYR	137	CD1	6.315661
113	1DK0	HIS	83	C	5.875345
114	1DK0	HIS	83	CA	5.309550
115	1DK0	HIS	83	N	6.515875
116	1DK0	HIS	32	O	5.920129

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
117	1DK0	THR	33	N	6.991008
118	1DK0	SER	42	O	6.312383
119	1DK0	SER	42	C	6.937601
120	1DK0	HIS	32	CA	6.464415
121	1DK0	THR	84	N	6.799510
122	1DK0	SER	42	CA	6.419147
123	1DK0	HIS	83	ND1	3.985590
124	1DK0	HIS	83	CE1	4.767730
125	1DK0	HIS	83	CB	4.746551
126	1DK0	LEU	77	CD1	5.795751
127	1DK0	HIS	32	C	6.271135
128	1DK0	LEU	77	O	6.856344
129	1DK0	LEU	77	CA	6.468919
130	1DK0	LEU	77	N	6.888315
131	1DK0	ASN	41	O	6.870425
132	1DK0	HIS	32	NE2	2.123754
133	1DK0	TYR	75	OH	2.104736
134	1DK0	TYR	75	CZ	3.011905
135	1DK0	TYR	75	CE2	3.827799
136	1DK0	TYR	75	CE1	3.681995
137	1DK0	TYR	75	CD2	4.982425
138	1DKH	HIS	83	C	5.475302
139	1DKH	HIS	32	NE2	2.724049
140	1DKH	VAL	37	CG2	5.406826
141	1DKH	VAL	37	CG1	5.465432
142	1DKH	VAL	37	CB	6.056663
143	1DKH	MET	140	SD	6.766447
144	1DKH	HIS	32	CD2	3.417608
145	1DKH	LEU	77	CD1	5.235716
146	1DKH	LEU	77	CG	6.605671
147	1DKH	LEU	77	CB	6.797675
148	1DKH	LEU	77	O	6.249675
149	1DKH	LEU	77	C	6.847101
150	1DKH	MET	140	CE	6.272749
151	1DKH	HIS	32	CG	4.691025

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
152	1DKH	TYR	75	OH	2.627310
153	1DKH	TYR	75	CZ	3.786304
154	1DKH	TYR	75	CE2	4.326754
155	1DKH	TYR	75	CE1	4.788814
156	1DKH	TYR	75	CD2	5.640713
157	1DKH	TYR	75	CD1	6.003591
158	1DKH	TYR	137	CE1	6.287721
159	1DKH	TYR	137	CD1	6.530572
160	1DKH	HIS	32	O	6.582967
161	1DKH	THR	84	N	6.267175
162	1DKH	HIS	83	NE2	6.220128
163	1DKH	HIS	83	CE1	5.346327
164	1DKH	HIS	83	CD2	5.826319
165	1DKH	HIS	32	CE1	3.857511
166	1DKH	HIS	83	CG	4.536138
167	1DKH	HIS	83	CB	3.988182
168	1DKH	HIS	83	O	5.472828
169	1DKH	HIS	32	CB	5.968356
170	1DKH	HIS	83	CA	4.987602
171	1DKH	HIS	83	N	6.204508
172	1DKH	HIS	32	CA	6.872067
173	1DKH	TYR	75	CG	6.376320
174	1DKH	HIS	32	ND1	4.892143
175	1DKH	HIS	32	C	6.888715
176	1DKH	LEU	77	CA	6.337690
177	1DKH	SER	42	O	6.070312
178	1DKH	HIS	83	ND1	4.180667
179	1ICC	PHE	58	CA	6.575948
180	1ICC	PHE	58	CZ	6.294185
181	1ICC	GLY	42	O	6.747263
182	1ICC	ALA	67	CB	6.085233
183	1ICC	GLY	41	O	6.760563
184	1ICC	GLY	41	C	6.125467
185	1ICC	PHE	58	CG	6.377746
186	1ICC	GLY	41	N	4.885432

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
187	1ICC	PHE	58	CE1	5.178997
188	1ICC	PRO	40	CG	6.377972
189	1ICC	GLY	42	N	6.567660
190	1ICC	HIS	39	CG	4.140159
191	1ICC	PRO	40	C	6.026885
192	1ICC	PRO	40	CA	6.297086
193	1ICC	PRO	40	N	5.739901
194	1ICC	HIS	39	NE2	2.123104
195	1ICC	HIS	39	CB	5.505745
196	1ICC	HIS	39	CE1	3.226539
197	1ICC	HIS	39	CD2	2.926974
198	1ICC	HIS	39	ND1	4.243412
199	1ICC	PHE	58	CD1	5.245447
200	1ICC	HIS	39	O	6.677095
201	1ICC	HIS	39	C	6.041067
202	1ICC	HIS	39	CA	5.995586
203	1ICC	HIS	63	NE2	2.158759
204	1ICC	GLY	41	CA	5.123949
205	1ICC	HIS	63	CD2	2.978584
206	1ICC	HIS	63	ND1	4.298568
207	1ICC	PHE	58	CB	6.924354
208	1ICC	HIS	63	CG	4.195708
209	1ICC	HIS	63	CB	5.559863
210	1ICC	HIS	63	CA	6.336951
211	1ICC	HIS	63	N	6.820816
212	1ICC	VAL	45	CG2	5.992035
213	1ICC	VAL	61	CG2	6.129882
214	1ICC	VAL	61	CG1	5.163116
215	1ICC	VAL	61	CB	5.887227
216	1ICC	PRO	40	CD	5.404471
217	1ICC	PHE	35	CZ	5.656220
218	1ICC	PHE	35	CE2	5.581214
219	1ICC	PHE	35	CE1	6.965375
220	1ICC	PHE	35	CD2	6.904462
221	1ICC	PHE	58	O	6.678997

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
222	1ICC	PRO	40	CB	6.254107
223	1ICC	LEU	46	CD1	6.354825
224	1ICC	LEU	46	CD2	5.305231
225	1ICC	LEU	46	CG	6.164095
226	1ICC	HIS	63	CE1	3.261015
227	1IPH	TYR	415	CD1	5.321445
228	1IPH	TYR	415	CG	5.753097
229	1IPH	TYR	415	CD2	5.155005
230	1IPH	PHE	214	CZ	4.709378
231	1IPH	VAL	199	CG1	5.331401
232	1IPH	VAL	199	CB	6.674711
233	1IPH	VAL	199	O	6.876508
234	1IPH	VAL	127	CG1	6.932478
235	1IPH	VAL	127	CB	6.007625
236	1IPH	PHE	214	CD2	6.247230
237	1IPH	PHE	214	CD1	6.328742
238	1IPH	ARG	411	NH2	4.309991
239	1IPH	ARG	411	NH1	5.763972
240	1IPH	ARG	411	CZ	4.644111
241	1IPH	ARG	411	NE	4.267373
242	1IPH	ARG	411	CD	5.225517
243	1IPH	ARG	411	CG	5.411208
244	1IPH	ARG	411	CA	6.789246
245	1IPH	PRO	393	CD	6.630299
246	1IPH	ARG	411	CB	6.156776
247	1IPH	PRO	393	CG	6.777688
248	1IPH	PHE	206	CZ	6.628821
249	1IPH	PHE	206	CE1	6.703106
250	1IPH	SER	414	OG	6.728176
251	1IPH	HIS	128	NE2	4.722708
252	1IPH	HIS	128	CE1	5.843978
253	1IPH	HIS	128	CD2	4.703907
254	1IPH	HIS	128	ND1	6.463455
255	1IPH	HIS	128	CG	5.886071
256	1IPH	HIS	128	CB	6.662541

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
257	1IPH	VAL	127	CG2	4.705092
258	1IPH	PHE	214	CE2	5.236705
259	1IPH	PHE	214	CE1	5.340604
260	1IPH	VAL	127	O	6.725119
261	1IPH	VAL	127	C	6.910519
262	1IPH	PHE	214	CG	6.743406
263	1IPH	TYR	415	CE1	4.124350
264	1IPH	TYR	415	OH	2.030382
265	1IPH	TYR	415	CZ	3.229706
266	1IPH	TYR	415	CE2	3.915944
267	1IPH	ASN	201	OD1	6.396844
268	1N45	THR	135	O	6.713859
269	1N45	HIS	25	NE2	1.986061
270	1N45	LEU	147	CD2	6.116868
271	1N45	LEU	147	CD1	5.813325
272	1N45	LEU	147	CG	6.417391
273	1N45	GLU	29	OE2	6.288778
274	1N45	HIS	25	CE1	2.963000
275	1N45	GLU	29	CD	6.437607
276	1N45	GLU	29	CG	6.106144
277	1N45	ALA	28	CB	6.981230
278	1N45	PHE	207	CD2	6.658300
279	1N45	GLY	143	O	6.659951
280	1N45	GLY	143	C	6.316242
281	1N45	GLY	143	CA	5.140301
282	1N45	GLY	143	N	5.415299
283	1N45	SER	142	CB	6.192592
284	1N45	SER	142	O	6.788654
285	1N45	SER	142	C	6.245701
286	1N45	SER	142	CA	6.873150
287	1N45	PHE	207	CZ	5.770283
288	1N45	PHE	207	CE2	5.499371
289	1N45	HIS	25	CD2	2.962420
290	1N45	HIS	25	ND1	4.055149
291	1N45	HIS	25	CG	4.092872

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
292	1N45	HIS	25	CB	5.516659
293	1N45	HIS	25	O	6.378513
294	1N45	HIS	25	C	6.673680
295	1N45	HIS	25	CA	6.276680
296	1N45	ASP	140	N	6.389011
297	1N45	GLY	139	C	5.233647
298	1N45	GLY	139	CA	4.866932
299	1N45	GLY	139	N	6.158972
300	1N45	LEU	138	O	6.569520
301	1N45	LEU	138	C	6.864677
302	1N45	GLY	139	O	4.745966
303	1P3T	PHE	181	CZ	6.065263
304	1P3T	PHE	181	CE2	5.883712
305	1P3T	ASP	27	N	6.593001
306	1P3T	CYS	113	O	6.881310
307	1P3T	VAL	26	CG1	6.716946
308	1P3T	ALA	121	CA	6.862152
309	1P3T	ALA	121	N	5.902582
310	1P3T	GLY	120	O	5.088974
311	1P3T	GLY	120	C	5.008701
312	1P3T	GLY	120	CA	4.368641
313	1P3T	GLY	120	N	4.908782
314	1P3T	LEU	119	CB	6.756164
315	1P3T	LEU	119	O	6.803831
316	1P3T	ASP	27	CA	6.459872
317	1P3T	LEU	119	C	6.123518
318	1P3T	LEU	119	CA	6.935993
319	1P3T	ASP	27	OD2	6.047626
320	1P3T	LEU	119	N	6.927501
321	1P3T	ASP	27	CG	6.315127
322	1P3T	ASN	118	N	6.625279
323	1P3T	SER	117	OG	6.830037
324	1P3T	SER	117	CB	5.457356
325	1P3T	SER	117	O	5.183198
326	1P3T	SER	117	C	5.447026

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
327	1P3T	SER	117	CA	4.802452
328	1P3T	SER	117	N	5.469435
329	1P3T	GLY	116	O	5.035610
330	1P3T	GLY	116	C	5.522926
331	1P3T	GLY	116	CA	6.653130
332	1P3T	HIS	23	NE2	2.123335
333	1P3T	HIS	23	CE1	3.040920
334	1P3T	HIS	23	CD2	3.170367
335	1P3T	HIS	23	ND1	4.185915
336	1P3T	HIS	23	CG	4.280040
337	1P3T	HIS	23	CB	5.709184
338	1P3T	HIS	23	O	5.852940
339	1P3T	HIS	23	C	6.366960
340	1P3T	HIS	23	CA	6.435673
341	1P3T	ASP	27	CB	5.923409
342	1QHU	HIS	213	N	6.818427
343	1QHU	GLU	225	CG	5.821887
344	1QHU	ASP	203	O	6.920576
345	1QHU	GLU	225	CD	6.788260
346	1QHU	GLU	225	CB	5.921903
347	1QHU	TYR	204	CE2	5.737836
348	1QHU	HIS	222	NE2	6.644323
349	1QHU	TYR	204	CD2	5.346169
350	1QHU	HIS	222	ND1	6.974400
351	1QHU	HIS	213	NE2	2.160954
352	1QHU	TYR	204	CG	6.385445
353	1QHU	TRP	171	CH2	6.047218
354	1QHU	TYR	204	O	6.162633
355	1QHU	TYR	204	C	6.870284
356	1QHU	TYR	204	CA	6.582455
357	1QHU	HIS	222	CE1	6.602165
358	1QHU	TRP	267	CH2	5.507890
359	1QHU	TRP	267	CZ3	5.473614
360	1QHU	TRP	267	CE3	6.485878
361	1QHU	TRP	267	CZ2	6.483137

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
362	1QHU	HIS	265	CA	6.677274
363	1QHU	ARG	214	CG	6.694055
364	1QHU	HIS	265	NE2	2.167072
365	1QHU	ARG	214	CB	6.175793
366	1QHU	ARG	214	N	6.896354
367	1QHU	SER	266	O	6.680148
368	1QHU	HIS	213	CE1	3.083658
369	1QHU	HIS	213	CD2	3.133678
370	1QHU	HIS	213	ND1	4.207582
371	1QHU	HIS	213	CG	4.250357
372	1QHU	HIS	213	CB	5.691865
373	1QHU	HIS	213	O	5.393894
374	1QHU	HIS	265	CE1	3.084628
375	1QHU	HIS	265	CD2	3.177235
376	1QHU	HIS	265	ND1	4.236295
377	1QHU	TYR	204	CB	6.591988
378	1QHU	HIS	213	CA	6.484866
379	1QHU	HIS	213	C	6.123380
380	1QHU	TRP	171	CZ3	6.247170
381	1QHU	HIS	265	CG	4.301112
382	1QHU	HIS	265	CB	5.757042
383	1QJS	ARG	214	N	6.770449
384	1QJS	HIS	213	CB	5.606479
385	1QJS	HIS	213	NE2	2.371645
386	1QJS	HIS	213	CE1	3.574877
387	1QJS	TYR	204	CD1	5.451236
388	1QJS	TYR	204	CG	6.449472
389	1QJS	TYR	204	CB	6.418390
390	1QJS	HIS	266	CB	5.985077
391	1QJS	TYR	204	C	6.653448
392	1QJS	TRP	268	CH2	5.757963
393	1QJS	TRP	268	CZ3	5.646631
394	1QJS	HIS	213	CD2	3.040290
395	1QJS	HIS	213	ND1	4.572235
396	1QJS	ASP	203	O	6.878437

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
397	1QJS	HIS	213	O	5.997544
398	1QJS	TYR	204	CE1	5.966506
399	1QJS	HIS	266	NE2	2.439885
400	1QJS	HIS	266	CE1	3.445671
401	1QJS	HIS	266	CD2	3.419325
402	1QJS	ARG	214	NH2	6.999397
403	1QJS	HIS	266	CG	4.605278
404	1QJS	GLU	226	OE1	6.866794
405	1QJS	HIS	266	CA	6.897887
406	1QJS	ARG	214	NH1	5.943540
407	1QJS	HIS	213	C	6.229975
408	1QJS	HIS	213	CA	6.547120
409	1QJS	ARG	214	CD	5.356812
410	1QJS	ARG	214	CZ	6.175478
411	1QJS	ARG	214	NE	5.917672
412	1QJS	TYR	204	O	6.252275
413	1QJS	HIS	266	ND1	4.597532
414	1QJS	SER	267	O	6.730283
415	1QJS	GLU	226	CD	6.990226
416	1QJS	GLU	226	CG	6.055635
417	1QJS	GLU	226	CB	5.949390
418	1QJS	HIS	213	CG	4.330243
419	1QJS	ARG	214	CG	6.580984
420	1QJS	TYR	204	CA	6.388720
421	1QJS	TRP	268	CZ2	6.847412
422	1QJS	TRP	171	CH2	6.207239
423	1QJS	TRP	171	CZ3	6.216160
424	1QJS	TRP	268	CE3	6.670834
425	1SI8	VAL	53	CB	5.947069
426	1SI8	PHE	140	CZ	4.567970
427	1SI8	PHE	140	CE2	5.104909
428	1SI8	PHE	140	CE1	5.129727
429	1SI8	PHE	140	CD2	6.057751
430	1SI8	PHE	140	CD1	6.083801
431	1SI8	PHE	140	CG	6.508549

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
432	1SI8	ARG	333	CA	6.916515
433	1SI8	ASN	127	ND2	6.475579
434	1SI8	ASN	127	OD1	6.570388
435	1SI8	PRO	315	CD	6.722802
436	1SI8	PRO	315	CG	6.356640
437	1SI8	VAL	125	CG1	5.290777
438	1SI8	VAL	125	CB	6.387496
439	1SI8	VAL	125	O	6.372424
440	1SI8	HIS	54	CD2	4.705726
441	1SI8	TYR	337	OH	1.764858
442	1SI8	TYR	337	CE2	3.708765
443	1SI8	TYR	337	CE1	3.793786
444	1SI8	TYR	337	CD2	5.002530
445	1SI8	ASN	127	CG	6.954157
446	1SI8	HIS	54	CB	6.658850
447	1SI8	TYR	337	CG	5.585404
448	1SI8	TYR	337	CZ	2.916787
449	1SI8	TYR	337	CD1	5.063792
450	1SI8	VAL	53	CG2	4.708814
451	1SI8	VAL	53	CG1	6.646728
452	1SI8	VAL	53	O	6.896312
453	1SI8	HIS	54	NE2	4.761949
454	1SI8	ARG	333	CG	5.432293
455	1SI8	HIS	54	CE1	5.832974
456	1SI8	HIS	54	CG	5.792320
457	1SI8	PHE	132	CZ	6.457172
458	1SI8	PHE	132	CE1	6.649313
459	1SI8	VAL	53	C	6.995423
460	1SI8	HIS	54	ND1	6.381505
461	1SI8	ARG	333	NH2	4.088012
462	1SI8	ARG	333	NH1	5.699736
463	1SI8	ARG	333	CZ	4.501158
464	1SI8	ARG	333	NE	4.109676
465	1SI8	ARG	333	CD	5.130376
466	1SI8	ARG	333	CB	6.103225

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
467	1SY2	HIS	59	NE2	1.991131
468	1SY2	HIS	59	CE1	2.969617
469	1SY2	HIS	59	CD2	3.008230
470	1SY2	PHE	68	CE1	6.731105
471	1SY2	HIS	59	ND1	4.093496
472	1SY2	HIS	59	CG	4.139204
473	1SY2	VAL	36	CG1	6.025207
474	1SY2	VAL	36	CB	6.934406
475	1SY2	PHE	68	CZ	5.479745
476	1SY2	PHE	68	CE2	5.463865
477	1SY2	PHE	68	CD2	6.718779
478	1SY2	TYR	58	O	6.964531
479	1SY2	LEU	57	CD1	6.145372
480	1SY2	ALA	42	CB	6.006055
481	1SY2	LEU	133	CD2	4.771642
482	1SY2	LEU	133	CD1	6.971913
483	1SY2	LEU	133	CG	6.296579
484	1SY2	LEU	133	CB	6.926720
485	1SY2	TYR	40	CE1	5.529416
486	1SY2	TYR	40	CD1	6.143980
487	1SY2	THR	121	CG2	6.333312
488	1SY2	HIS	59	CA	6.572801
489	1SY2	TYR	40	CZ	6.015462
490	1SY2	TYR	40	OH	5.862889
491	1SY2	LEU	123	CD2	5.102667
492	1SY2	HIS	59	CB	5.543230
493	1SY2	LEU	123	CD1	6.319238
494	1SY2	LEU	123	CG	6.093997
495	1SY2	LEU	123	CB	6.095758
496	1U9U	HIS	39	CG	4.206256
497	1U9U	LEU	46	CG	6.187550
498	1U9U	TYR	58	OH	6.699568
499	1U9U	TYR	58	CZ	6.326789
500	1U9U	GLY	42	N	6.680137
501	1U9U	VAL	45	CG2	6.942157

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
502	1U9U	VAL	45	CG1	6.058232
503	1U9U	TYR	58	CD1	5.273249
504	1U9U	TYR	58	CG	6.538044
505	1U9U	GLY	41	O	6.645878
506	1U9U	HIS	39	O	6.864918
507	1U9U	TYR	58	O	6.735663
508	1U9U	TYR	58	CA	6.913788
509	1U9U	HIS	39	C	6.191801
510	1U9U	GLY	41	C	6.113410
511	1U9U	GLY	41	CA	5.128111
512	1U9U	HIS	39	CA	6.111432
513	1U9U	GLY	41	N	5.006643
514	1U9U	GLY	42	O	6.699127
515	1U9U	PRO	40	CD	5.614395
516	1U9U	PRO	40	CG	6.488790
517	1U9U	PRO	40	CB	6.335580
518	1U9U	PRO	40	C	6.123416
519	1U9U	PRO	40	CA	6.448076
520	1U9U	PRO	40	N	5.886755
521	1U9U	HIS	39	NE2	2.043206
522	1U9U	HIS	39	CE1	3.048365
523	1U9U	TYR	58	CE1	5.142585
524	1U9U	ALA	67	CB	6.016697
525	1U9U	HIS	39	ND1	4.185334
526	1U9U	HIS	39	CB	5.603902
527	1U9U	HIS	63	NE2	2.014515
528	1U9U	HIS	63	CE1	3.015075
529	1U9U	HIS	63	CD2	3.029380
530	1U9U	HIS	63	ND1	4.158058
531	1U9U	HIS	63	CG	4.183993
532	1U9U	HIS	63	CB	5.583220
533	1U9U	HIS	63	CA	6.401253
534	1U9U	PHE	35	CZ	5.951020
535	1U9U	PHE	35	CE1	5.597399
536	1U9U	PHE	35	CD1	6.735596

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
537	1U9U	VAL	61	CG2	5.482450
538	1U9U	VAL	61	CG1	6.660130
539	1U9U	HIS	39	CD2	3.048436
540	1U9U	VAL	61	CB	6.348508
541	1U9U	HIS	63	N	6.957491
542	1U9U	LEU	46	CD2	5.296413
543	1U9U	LEU	46	CD1	6.392325
544	1VGI	ASP	140	N	6.566393
545	1VGI	GLY	139	O	4.909939
546	1VGI	GLY	139	C	5.283546
547	1VGI	GLY	139	CA	4.648608
548	1VGI	GLY	139	N	5.779788
549	1VGI	LEU	138	C	6.281721
550	1VGI	THR	135	O	6.883314
551	1VGI	GLU	29	OE2	6.243035
552	1VGI	GLU	29	OE1	5.985395
553	1VGI	GLU	29	CD	6.086993
554	1VGI	GLU	29	CG	6.516177
555	1VGI	GLU	29	CB	5.743143
556	1VGI	LEU	138	O	5.939267
557	1VGI	GLU	29	CA	6.608512
558	1VGI	GLU	29	N	6.775782
559	1VGI	PHE	207	CD2	6.972948
560	1VGI	PHE	207	CE2	5.769644
561	1VGI	PHE	207	CZ	5.974394
562	1VGI	GLY	144	N	5.974807
563	1VGI	GLY	143	O	6.628912
564	1VGI	GLY	143	C	5.710274
565	1VGI	GLY	143	CA	4.511340
566	1VGI	GLY	143	N	4.268353
567	1VGI	SER	142	OG	5.504225
568	1VGI	SER	142	CB	4.695014
569	1VGI	SER	142	O	6.489063
570	1VGI	SER	142	C	5.437356
571	1VGI	SER	142	CA	5.720043

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
572	1VGI	SER	142	N	6.355931
573	1VGI	HIS	25	NE2	2.129611
574	1VGI	HIS	25	CE1	3.138380
575	1VGI	HIS	25	CD2	3.080753
576	1VGI	HIS	25	ND1	4.235989
577	1VGI	HIS	25	CG	4.243468
578	1VGI	HIS	25	CB	5.650238
579	1VGI	HIS	25	O	6.255406
580	1VGI	HIS	25	C	6.671689
581	1VGI	HIS	25	CA	6.410085
582	1ZVI	TRP	409	NE1	4.390030
583	1ZVI	TRP	409	CD2	6.307480
584	1ZVI	TRP	409	CD1	5.061980
585	1ZVI	TRP	409	CG	6.187796
586	1ZVI	ALA	412	O	6.765352
587	1ZVI	GLY	417	O	5.991773
588	1ZVI	ALA	412	CB	6.197408
589	1ZVI	TRP	409	CH2	6.817691
590	1ZVI	GLY	586	N	6.997972
591	1ZVI	TRP	409	CZ2	5.585668
592	1ZVI	TRP	409	CE2	5.271278
593	1ZVI	PHE	584	CD1	6.145291
594	1ZVI	GLY	417	CA	5.225372
595	1ZVI	ARG	418	CG	6.178065
596	1ZVI	VAL	416	C	5.918608
597	1ZVI	ARG	418	CA	6.675410
598	1ZVI	ARG	418	N	5.925158
599	1ZVI	GLY	417	C	5.585365
600	1ZVI	GLY	417	N	4.817420
601	1ZVI	VAL	416	CG1	6.132313
602	1ZVI	VAL	416	CB	6.790595
603	1ZVI	GLU	592	OE1	6.601349
604	1ZVI	VAL	416	CA	6.037081
605	1ZVI	TRP	587	O	6.843603
606	1ZVI	CYS	415	SG	2.308670

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
607	1ZVI	CYS	415	CB	3.198440
608	1ZVI	CYS	415	O	5.568409
609	1ZVI	CYS	415	C	4.775958
610	1ZVI	CYS	415	CA	4.044635
611	1ZVI	CYS	415	N	5.194890
612	1ZVI	VAL	416	N	4.925378
613	1ZVI	ARG	414	O	5.732163
614	1ZVI	ARG	414	C	5.866689
615	1ZVI	PHE	584	CZ	6.329761
616	1ZVI	PHE	584	CE1	5.554874
617	2BHJ	TRP	188	CZ2	6.222844
618	2BHJ	TRP	188	CE2	5.893418
619	2BHJ	TRP	188	NE1	5.125246
620	2BHJ	PHE	363	CE1	5.474852
621	2BHJ	TRP	188	CD2	6.779083
622	2BHJ	TRP	188	CD1	5.641795
623	2BHJ	TRP	188	CG	6.631906
626	2BHJ	ILE	195	CA	6.453869
630	2BHJ	ARG	197	CG	6.260527
635	2BHJ	TRP	366	O	6.764735
637	2BHJ	GLY	365	C	6.979700
638	2BHJ	GLY	365	CA	6.306240
639	2BHJ	GLY	365	N	6.566821
640	2BHJ	VAL	346	CG2	6.643571
641	2BHJ	ARG	197	CA	6.757059
642	2BHJ	ARG	193	O	5.497250
643	2BHJ	ARG	197	N	5.646104
644	2BHJ	ARG	193	C	5.992947
645	2BHJ	GLY	196	C	5.839840
646	2BHJ	GLY	196	CA	4.990296
647	2BHJ	GLY	196	N	4.924861
648	2BHJ	PHE	363	CZ	6.572774
649	2BHJ	ILE	195	CG1	6.874262
650	2BHJ	GLY	196	O	6.913416
651	2BHJ	PHE	363	CD1	5.892929

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
652	2BHJ	ILE	195	C	6.137234
653	2BHJ	ALA	191	CB	6.261711
655	2BHJ	ILE	195	N	5.399846
656	2BHJ	ASN	364	C	6.955669
657	2BHJ	CYS	194	SG	2.550330
658	2BHJ	CYS	194	CB	3.455701
659	2BHJ	CYS	194	O	5.801798
660	2BHJ	CYS	194	C	5.116600
661	2BHJ	CYS	194	CA	4.401892
662	2BHJ	CYS	194	N	5.598660
663	2CJ0	PRO	30	CA	6.413160
664	2CJ0	PRO	30	N	5.305511
665	2CJ0	PRO	28	O	6.087495
666	2CJ0	LEU	32	CG	5.201324
667	2CJ0	PHE	57	CZ	5.997218
668	2CJ0	PHE	57	CE2	6.943680
669	2CJ0	PHE	57	CE1	6.513037
670	2CJ0	PRO	28	C	6.167848
671	2CJ0	LEU	32	CB	6.048838
672	2CJ0	CYS	29	SG	2.332979
673	2CJ0	PHE	186	CZ	5.733194
674	2CJ0	PHE	186	CE2	4.498737
675	2CJ0	PHE	186	CE1	6.809006
676	2CJ0	PHE	186	CD2	4.600610
677	2CJ0	PHE	186	CD1	6.871748
678	2CJ0	PHE	186	CG	5.885035
679	2CJ0	PHE	186	CB	6.436140
680	2CJ0	ALA	71	CB	6.531120
681	2CJ0	GLU	183	CG	5.000890
682	2CJ0	CYS	29	O	5.828148
683	2CJ0	PHE	103	CZ	5.720504
684	2CJ0	PHE	103	CE2	6.636227
685	2CJ0	PHE	103	CE1	5.717665
686	2CJ0	PHE	103	CD1	6.657126
687	2CJ0	GLU	183	CB	6.148012

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
688	2CJ0	LEU	32	CD2	6.182563
689	2CJ0	LEU	32	CD1	5.205139
690	2CJ0	GLU	183	OE2	4.813794
691	2CJ0	LEU	32	N	5.473763
692	2CJ0	GLU	183	OE1	6.305254
693	2CJ0	TRP	213	CZ2	6.764355
694	2CJ0	GLU	183	CD	5.296878
695	2CJ0	LEU	32	CA	6.431553
696	2CJ0	ALA	31	CB	4.801695
697	2CJ0	GLU	183	CA	6.731475
698	2CJ0	ALA	31	C	6.117251
699	2CJ0	ALA	31	CA	5.615654
700	2CJ0	ALA	31	N	5.228885
701	2CJ0	PRO	30	CD	4.998710
703	2CJ0	PRO	30	CG	5.851687
704	2CJ0	PRO	30	CB	6.887230
706	2CJ0	PRO	30	C	6.306888
707	2CJ0	CYS	29	CB	3.353759
709	2CJ0	CYS	29	C	5.082226
710	2CJ0	CYS	29	CA	4.298322
711	2CJ0	CYS	29	N	5.449996
713	2CN4	TYR	137	CE1	5.999989
714	2CN4	LEU	77	CD1	5.872843
715	2CN4	LEU	77	O	6.708273
716	2CN4	TYR	75	CD1	4.937744
717	2CN4	LEU	77	C	6.957343
718	2CN4	LEU	77	CA	6.369264
719	2CN4	LEU	77	N	6.836199
720	2CN4	MET	140	SD	6.431033
721	2CN4	TYR	75	OH	1.967570
722	2CN4	TYR	75	CE2	3.773859
723	2CN4	TYR	75	CG	5.495449
724	2CN4	TYR	75	CB	6.949941
725	2CN4	TYR	75	CE1	3.696255
726	2CN4	THR	84	N	6.804573

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
727	2CN4	HIS	83	NE2	5.663518
728	2CN4	HIS	83	CE1	4.646133
729	2CN4	HIS	83	CD2	5.660304
730	2CN4	HIS	83	ND1	3.832308
731	2CN4	HIS	83	CG	4.590615
732	2CN4	HIS	83	O	5.774314
733	2CN4	HIS	83	C	5.865981
734	2CN4	HIS	83	CA	5.304336
735	2CN4	HIS	83	N	6.539553
736	2CN4	TYR	75	CD2	4.987756
737	2CN4	TYR	137	CD1	6.285768
738	2CN4	MET	140	CE	5.201521
739	2CN4	TYR	55	OH	6.806239
740	2CN4	HIS	83	CB	4.641684
741	2CN4	TYR	75	CZ	2.951862
742	2CPO	PHE	103	CD1	6.975511
743	2CPO	GLU	183	OE2	4.939676
744	2CPO	GLU	183	OE1	6.335940
745	2CPO	GLU	183	CD	5.349221
746	2CPO	GLU	183	CG	5.054924
747	2CPO	GLU	183	CB	6.268234
748	2CPO	PHE	186	CE2	4.603752
749	2CPO	GLU	183	CA	6.849042
750	2CPO	PHE	186	CE1	6.837423
751	2CPO	PRO	30	CD	5.233183
752	2CPO	PRO	30	CG	5.856242
753	2CPO	PRO	30	CB	6.905368
754	2CPO	ALA	71	CB	6.539227
755	2CPO	PHE	57	CZ	6.204651
756	2CPO	PHE	57	CE1	6.743175
757	2CPO	PRO	30	C	6.340386
758	2CPO	PRO	30	CA	6.422284
759	2CPO	LEU	32	CD1	5.464368
760	2CPO	LEU	32	CD2	6.378116
761	2CPO	LEU	32	CG	5.367063

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
762	2CPO	LEU	32	CB	6.113132
763	2CPO	LEU	32	CA	6.537572
764	2CPO	ALA	31	CB	4.859749
765	2CPO	ALA	31	C	6.209249
766	2CPO	ALA	31	CA	5.676009
767	2CPO	ALA	31	N	5.275484
768	2CPO	PRO	30	N	5.345663
769	2CPO	CYS	29	SG	2.280053
770	2CPO	CYS	29	CB	3.456969
771	2CPO	CYS	29	O	5.849326
772	2CPO	CYS	29	C	5.117841
773	2CPO	CYS	29	CA	4.399908
774	2CPO	CYS	29	N	5.557198
775	2CPO	LEU	32	N	5.618095
776	2CPO	PHE	186	CZ	5.795715
777	2CPO	PRO	28	O	5.903420
778	2CPO	PRO	28	C	6.132974
779	2CPO	PHE	186	CD2	4.688355
780	2CPO	PHE	186	CD1	6.888712
781	2CPO	PHE	186	CG	5.928563
782	2CPO	PHE	186	CB	6.495107
783	2CPO	PHE	103	CZ	5.900386
784	2CPO	PHE	103	CE2	6.595274
785	2CPO	PHE	103	CE1	6.115996
786	2E2Y	ILE	68	CA	6.025953
787	2E2Y	HIS	93	NE2	2.147339
788	2E2Y	HIS	93	CE1	3.084295
789	2E2Y	HIS	93	ND1	4.218828
790	2E2Y	ILE	68	CD1	4.615037
791	2E2Y	HIS	93	CB	5.719846
792	2E2Y	ILE	68	CG1	4.409347
793	2E2Y	ILE	68	CB	5.618411
794	2E2Y	HIS	93	CA	6.508268
795	2E2Y	HIS	93	N	6.974609
796	2E2Y	SER	92	OG	6.454585

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
797	2E2Y	ILE	68	N	6.587345
798	2E2Y	THR	67	CG2	6.891096
799	2E2Y	LEU	89	CD2	6.840761
800	2E2Y	LEU	89	CD1	5.350779
801	2E2Y	TRP	43	CH2	4.785277
802	2E2Y	TRP	43	CZ3	5.726918
803	2E2Y	TRP	43	CZ2	4.837758
804	2E2Y	TRP	43	CE3	6.592627
805	2E2Y	TRP	43	CE2	5.822864
806	2E2Y	LEU	89	CG	6.312412
807	2E2Y	ASP	64	O	6.865050
808	2E2Y	TRP	43	NE1	6.512078
809	2E2Y	HIS	97	NE2	5.536711
810	2E2Y	TRP	43	CD2	6.641236
811	2E2Y	ILE	107	CD1	6.704700
812	2E2Y	HIS	93	CD2	3.169440
813	2E2Y	ILE	99	CG1	5.522935
814	2E2Y	HIS	93	CG	4.293654
815	2E2Y	ILE	68	CG2	5.846267
816	2E2Y	ILE	99	CD1	6.203939
817	2E2Y	ILE	99	CG2	6.408774
818	2E2Y	ILE	99	CB	6.387531
819	2E2Y	HIS	97	CE1	6.449086
820	2E2Y	LEU	104	CD2	6.384225
821	2E2Y	HIS	97	CD2	5.024194
822	2E2Y	HIS	97	ND1	6.574172
823	2E2Y	HIS	97	CG	5.764004
824	2E2Y	HIS	97	CB	6.154168
825	2FC2	TRP	56	CG	6.458449
834	2FC2	TRP	56	CZ2	5.815614
835	2FC2	TRP	56	CE2	5.533414
836	2FC2	TRP	56	NE1	4.699520
837	2FC2	TRP	56	CD2	6.562358
838	2FC2	TRP	56	CD1	5.358495
839	2FC2	ILE	63	N	5.228967

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
840	2FC2	CYS	62	SG	2.435575
841	2FC2	CYS	62	CB	3.536192
842	2FC2	CYS	62	O	5.978278
843	2FC2	CYS	62	C	5.144583
844	2FC2	CYS	62	CA	4.362565
845	2FC2	CYS	62	N	5.440083
846	2FC2	ARG	61	O	6.037753
847	2FC2	ARG	61	C	6.107353
849	2FC2	ILE	214	CD1	6.545905
850	2FC2	PHE	231	CZ	6.507050
851	2FC2	TRP	234	O	6.837576
852	2FC2	SER	59	CB	6.581787
853	2FC2	GLY	233	CA	6.467865
854	2FC2	GLY	233	N	6.567286
855	2FC2	PHE	231	CD1	6.261662
856	2FC2	ARG	65	N	6.375567
857	2FC2	GLY	64	O	6.600001
858	2FC2	GLY	64	C	6.081704
859	2FC2	GLY	64	CA	5.643363
860	2FC2	GLY	64	N	5.205832
861	2FC2	ILE	63	CG2	6.571768
862	2FC2	PHE	231	CE1	5.620466
863	2FC2	ILE	63	C	6.279963
864	2FC2	ILE	63	CA	6.344814
865	2FC2	ARG	65	CG	6.543414
866	2IIZ	VAL	228	CG1	5.347881
867	2IIZ	ARG	242	CD	4.829683
868	2IIZ	ARG	242	CG	6.171953
869	2IIZ	ARG	242	NE	5.250492
870	2IIZ	HIS	224	NE2	2.083556
871	2IIZ	VAL	228	CB	5.630430
872	2IIZ	ASP	151	OD1	4.711695
873	2IIZ	LEU	255	CD2	6.075868
874	2IIZ	ASP	151	CG	5.736038
875	2IIZ	ILE	225	CG1	6.959216

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
876	2IIZ	HIS	224	ND1	4.196756
877	2IIZ	ILE	225	N	6.765893
878	2IIZ	HIS	224	CD2	2.916346
879	2IIZ	HIS	224	CG	4.113269
880	2IIZ	HIS	224	CB	5.483611
881	2IIZ	HIS	224	O	6.074125
883	2IIZ	ASP	151	OD2	6.083437
884	2IIZ	HIS	224	C	6.285813
885	2IIZ	LEU	286	CD2	5.566800
886	2IIZ	ILE	225	CD1	5.566335
888	2IIZ	ASP	284	OD2	6.598336
889	2IIZ	ASP	151	CB	6.913658
890	2IIZ	HIS	224	CA	6.479182
891	2IIZ	HIS	224	CE1	3.169809
892	2IIZ	PHE	257	CZ	5.892569
893	2IIZ	PHE	257	CE1	4.932157
894	2IIZ	PHE	257	CD1	5.448107
895	2IIZ	PHE	257	CG	6.723349
896	2IIZ	ARG	242	CZ	5.007478
897	2IIZ	ARG	242	NH2	5.941234
898	2IIZ	ARG	242	NH1	4.220492
899	2IIZ	VAL	228	CG2	4.969134
900	2IPS	HIS	351	CA	5.749235
901	2IPS	HIS	351	N	5.858503
902	2IPS	GLY	350	C	6.712596
903	2IPS	GLN	105	CD	5.606023
904	2IPS	HIS	351	ND1	4.080454
905	2IPS	HIS	351	CB	5.415193
908	2IPS	HIS	351	CE1	3.037140
909	2IPS	LEU	433	CD2	4.521870
910	2IPS	ARG	348	NH1	6.543196
911	2IPS	ARG	348	NE	6.592648
912	2IPS	ARG	348	CG	5.980233
913	2IPS	ARG	348	CB	5.960582
914	2IPS	ARG	348	O	6.358253

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
915	2IPS	ARG	348	C	6.696090
916	2IPS	ARG	348	CA	6.098489
917	2IPS	HIS	109	NE2	5.382487
918	2IPS	HIS	109	CE1	6.247737
919	2IPS	HIS	109	CD2	6.143644
920	2IPS	GLN	105	NE2	4.751823
921	2IPS	ARG	348	CZ	6.859686
922	2IPS	LEU	433	CD1	5.160410
923	2IPS	HIS	351	CD2	2.856701
924	2IPS	HIS	351	CG	4.029645
925	2IPS	ASP	108	OD2	6.127171
926	2IPS	ARG	348	CD	5.940936
927	2IPS	LEU	433	CB	6.783302
928	2IPS	ASP	108	OD1	5.467499
929	2IPS	GLU	258	OE2	6.284643
930	2IPS	GLU	258	OE1	6.107822
931	2IPS	GLU	258	CD	6.256175
932	2IPS	ASP	108	CG	6.018289
933	2IPS	GLU	258	CG	6.906953
934	2IPS	GLN	105	OE1	6.758873
935	2IPS	GLN	105	CG	5.451591
936	2IPS	GLN	105	CB	6.437183
937	2IPS	VAL	354	CG2	6.655642
938	2IPS	LEU	417	CD1	6.682821
939	2IPS	LEU	417	CD2	6.901804
940	2IPS	ASN	437	ND2	6.083718
941	2IPS	ASN	437	OD1	6.134033
942	2IPS	ASN	437	CG	6.613187
943	2IPS	GLN	105	CA	6.884046
944	2IPS	HIS	351	NE2	1.979467
945	2IPS	LEU	433	CG	5.368566
946	2J0P	ILE	255	CD1	5.544619
947	2J0P	ILE	255	CG1	6.850121
948	2J0P	HIS	196	ND1	4.052531
949	2J0P	PHE	199	CE1	6.621060

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
950	2J0P	VAL	195	CG2	5.617753
951	2J0P	PHE	246	CE1	5.416275
952	2J0P	VAL	195	CB	6.997294
953	2J0P	HIS	196	NE2	1.995959
954	2J0P	HIS	196	CE1	2.913044
955	2J0P	HIS	196	CD2	3.047082
956	2J0P	HIS	196	CG	4.149956
957	2J0P	PHE	199	CZ	6.315753
958	2J0P	HIS	196	CB	5.582205
959	2J0P	HIS	196	CA	6.299600
960	2J0P	HIS	196	N	6.442225
961	2J0P	PHE	246	CE2	6.985655
962	2J0P	ASP	194	OD2	6.862392
963	2J0P	PHE	246	CZ	5.694124
964	2J0P	ARG	102	NH2	6.037140
965	2J0P	ARG	102	NH1	4.561750
966	2J0P	ARG	102	CZ	4.755083
967	2J0P	ARG	102	NE	3.944642
968	2J0P	ARG	102	CD	4.681022
969	2J0P	ARG	102	CG	4.986154
970	2J0P	ARG	102	CB	6.050972
971	2J0P	PHE	246	CD1	6.523961
972	2J0P	MET	244	CE	6.821994
973	2J18	PRO	30	C	6.327097
974	2J18	GLU	183	OE2	4.947637
975	2J18	GLU	183	OE1	6.248705
976	2J18	GLU	183	CD	5.296484
977	2J18	GLU	183	CG	4.971319
978	2J18	GLU	183	CB	6.127612
979	2J18	PRO	30	CA	6.400263
980	2J18	GLU	183	CA	6.743073
981	2J18	PRO	30	N	5.267359
982	2J18	CYS	29	SG	2.327225
983	2J18	TRP	213	CZ2	6.782850
984	2J18	LEU	32	CD2	6.145673

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
985	2J18	LEU	32	CD1	5.249746
986	2J18	CYS	29	O	5.805364
987	2J18	LEU	32	CG	5.192432
988	2J18	LEU	32	CB	6.073104
989	2J18	LEU	32	CA	6.427634
990	2J18	LEU	32	N	5.474246
991	2J18	PRO	30	CD	4.944045
992	2J18	CYS	29	CA	4.267326
993	2J18	PRO	30	CG	5.811047
994	2J18	PRO	30	CB	6.868480
995	2J18	ALA	31	CB	4.824723
996	2J18	CYS	29	CB	3.312756
997	2J18	CYS	29	N	5.406223
998	2J18	PHE	103	CZ	5.737781
999	2J18	PHE	57	CE1	6.580041
1000	2J18	PHE	103	CE2	6.552953
1001	2J18	PRO	28	O	6.068358
1002	2J18	PRO	28	C	6.137689
1003	2J18	PHE	103	CD1	6.785377
1004	2J18	ALA	31	C	6.121039
1005	2J18	ALA	31	CA	5.629992
1006	2J18	PHE	57	CZ	6.059994
1007	2J18	CYS	29	C	5.040428
1008	2J18	PHE	103	CE1	5.867260
1009	2J18	PHE	57	CE2	6.963378
1010	2J18	ALA	31	N	5.252748
1011	2J18	PHE	186	CZ	5.827151
1012	2J18	PHE	186	CE2	4.556892
1013	2J18	ALA	71	CB	6.477348
1014	2J18	PHE	186	CE1	6.896912
1015	2J18	PHE	186	CD2	4.616209
1016	2J18	PHE	186	CD1	6.919913
1017	2J18	PHE	186	CG	5.911162
1018	2J18	PHE	186	CB	6.451495
1019	2O6P	VAL	119	CG2	6.077404

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1020	2O6P	VAL	119	CG1	6.110981
1021	2O6P	VAL	119	CB	6.341395
1022	2O6P	TYR	132	CD1	4.915283
1023	2O6P	ALA	49	CA	6.635661
1024	2O6P	ALA	49	N	6.076465
1025	2O6P	ILE	48	CD1	4.864651
1026	2O6P	ILE	48	CG2	3.754376
1027	2O6P	TYR	136	CE2	4.244835
1028	2O6P	TYR	136	CE1	5.540031
1029	2O6P	ILE	48	O	6.128135
1030	2O6P	ILE	48	C	5.861636
1031	2O6P	ILE	48	CA	5.831651
1032	2O6P	ILE	48	N	6.659443
1033	2O6P	TYR	136	OH	3.981181
1034	2O6P	HIS	134	CD2	6.249883
1035	2O6P	HIS	134	CG	6.658817
1036	2O6P	HIS	134	CB	6.581079
1037	2O6P	ILE	48	CG1	5.280432
1038	2O6P	TYR	132	OH	2.048273
1039	2O6P	TYR	132	CZ	3.029479
1040	2O6P	ILE	48	CB	4.547451
1041	2O6P	TYR	132	CE2	3.989407
1042	2O6P	TYR	132	CE1	3.649141
1043	2O6P	TYR	132	CD2	5.171507
1044	2O6P	TYR	132	CG	5.582168
1045	2O6P	TYR	136	CD2	5.259598
1046	2O6P	ILE	121	CD1	6.852081
1047	2O6P	TYR	136	CG	6.236712
1048	2O6P	TYR	136	CZ	4.436833
1049	2O6P	TYR	52	OH	6.883091
1050	2O6P	TYR	52	CE2	6.481230
1051	2O6P	TYR	136	CD1	6.340717
1052	2Q6N	GLY	299	N	6.518431
1053	2Q6N	ALA	298	CB	4.749119
1054	2Q6N	ALA	298	O	6.101358

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1055	2Q6N	ALA	298	C	6.018864
1056	2Q6N	ALA	298	CA	5.818802
1057	2Q6N	ALA	442	CB	6.935846
1058	2Q6N	ILE	363	CD1	6.720194
1059	2Q6N	ILE	435	C	6.428855
1062	2Q6N	ILE	363	CG1	6.869433
1063	2Q6N	PHE	429	CE1	6.200513
1064	2Q6N	PHE	429	CD1	5.568040
1065	2Q6N	PHE	429	CG	6.421549
1066	2Q6N	PHE	429	CB	6.289117
1067	2Q6N	PHE	429	O	6.015390
1068	2Q6N	PHE	429	C	6.622543
1069	2Q6N	PHE	429	CA	6.228656
1070	2Q6N	ILE	114	CD1	6.560571
1071	2Q6N	PRO	428	O	6.945175
1072	2Q6N	THR	302	CB	5.787195
1073	2Q6N	GLY	438	CA	5.530851
1075	2Q6N	THR	302	CG2	6.196351
1077	2Q6N	CYS	436	CB	3.412142
1078	2Q6N	GLU	439	N	5.919996
1079	2Q6N	GLY	438	O	6.147005
1080	2Q6N	GLY	438	C	5.742671
1082	2Q6N	GLU	439	CA	6.620933
1083	2Q6N	GLY	438	N	5.042187
1086	2Q6N	LEU	437	CB	6.344581
1088	2Q6N	LEU	437	C	6.077450
1089	2Q6N	LEU	437	CA	6.051221
1090	2Q6N	LEU	437	N	4.986629
1091	2Q6N	CYS	436	SG	2.272461
1092	2Q6N	THR	302	OG1	5.261641
1093	2Q6N	CYS	436	O	5.714731
1094	2Q6N	CYS	436	C	4.893650
1095	2Q6N	CYS	436	CA	4.182302
1096	2Q6N	CYS	436	N	5.358535
1097	2Q6N	ILE	435	O	6.634527

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1098	2R7A	GLN	253	OE1	5.564728
1099	2R7A	LEU	257	CD2	6.219739
1100	2R7A	TYR	67	CE2	4.383000
1101	2R7A	LEU	257	CD1	4.400343
1102	2R7A	TYR	67	CE1	3.419765
1103	2R7A	LEU	257	CG	5.709105
1104	2R7A	GLY	170	CA	6.235709
1105	2R7A	GLY	170	N	5.608906
1106	2R7A	ALA	169	CB	3.961766
1107	2R7A	ALA	169	O	5.437785
1108	2R7A	ALA	169	C	5.238544
1109	2R7A	ALA	169	CA	5.115560
1110	2R7A	ALA	169	N	6.361366
1111	2R7A	TRP	68	CZ2	6.285840
1112	2R7A	TYR	67	CD1	4.728948
1113	2R7A	TYR	67	CG	5.632054
1114	2R7A	LEU	167	CD1	6.804120
1115	2R7A	LEU	167	CG	6.791967
1116	2R7A	LEU	257	CB	5.908137
1117	2R7A	TRP	68	NE1	5.647304
1118	2R7A	TRP	68	CD1	6.518906
1119	2R7A	TYR	67	OH	2.299557
1120	2R7A	TYR	67	CZ	3.183906
1121	2R7A	GLN	253	CD	6.597577
1122	2R7A	TYR	67	CD2	5.472719
1123	2R7A	TRP	68	CE2	6.316415
1124	2R7A	LEU	167	CD2	5.928353
1125	2R7A	THR	52	CG2	4.925867
1126	2R7A	THR	52	CB	6.038417
1127	2R7A	THR	52	CA	6.872261
1128	2SPL	HIS	93	N	6.994165
1129	2SPL	SER	92	OG	6.650791
1130	2SPL	HIS	64	NE2	5.038259
1131	2SPL	HIS	64	CE1	4.912606
1132	2SPL	HIS	64	CD2	6.439022

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1133	2SPL	HIS	64	ND1	6.172233
1134	2SPL	HIS	64	CG	6.883278
1135	2SPL	PHE	43	CD2	6.365638
1136	2SPL	LEU	89	CD2	5.552852
1137	2SPL	LEU	89	CD1	6.956336
1138	2SPL	LEU	89	CG	6.830744
1139	2SPL	HIS	97	CB	6.284240
1140	2SPL	PHE	29	CZ	5.942149
1141	2SPL	PHE	29	CE1	6.316924
1142	2SPL	ILE	99	CD1	6.105261
1143	2SPL	ILE	99	CG2	6.554861
1144	2SPL	ILE	99	CG1	5.648982
1145	2SPL	PHE	43	CZ	5.252572
1146	2SPL	ILE	99	CB	6.583026
1147	2SPL	HIS	93	NE2	2.250800
1148	2SPL	PHE	43	CE2	5.171565
1150	2SPL	PHE	43	CE1	6.470892
1152	2SPL	HIS	97	CE1	6.582138
1153	2SPL	HIS	97	CD2	5.019365
1154	2SPL	HIS	97	ND1	6.645861
1155	2SPL	HIS	97	CG	5.854444
1156	2SPL	ILE	107	CD1	6.505472
1157	2SPL	LEU	104	CD2	6.518599
1158	2SPL	VAL	68	CG1	5.450572
1159	2SPL	VAL	68	CG2	4.726055
1160	2SPL	VAL	68	CA	6.468528
1161	2SPL	HIS	97	NE2	5.600465
1162	2SPL	HIS	93	CE1	3.180650
1163	2SPL	VAL	68	CB	5.746902
1164	2SPL	HIS	93	CD2	3.237413
1165	2SPL	HIS	93	ND1	4.311525
1166	2SPL	HIS	93	CG	4.404178
1167	2SPL	HIS	93	CB	5.753593
1168	2SPL	HIS	93	CA	6.496039
1169	2VEB	VAL	89	CG1	5.917494

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1170	2VEB	ILE	116	CG2	6.182483
1173	2VEB	PHE	74	CZ	5.980082
1174	2VEB	PHE	74	CE2	6.347131
1175	2VEB	PHE	74	CE1	6.888940
1176	2VEB	ILE	137	CD1	5.210730
1177	2VEB	ILE	137	CG2	6.657078
1178	2VEB	ILE	137	CG1	6.593755
1179	2VEB	PHE	145	CE2	6.316550
1180	2VEB	PHE	145	CD2	6.105756
1181	2VEB	PHE	93	CE2	5.450832
1182	2VEB	PHE	93	CE1	5.557580
1183	2VEB	PHE	93	CD2	5.744187
1184	2VEB	PHE	93	CZ	5.331525
1185	2VEB	PHE	93	CD1	5.865122
1186	2VEB	PHE	93	CB	6.757747
1187	2VEB	HIS	120	NE2	2.127885
1188	2VEB	HIS	120	CE1	3.089174
1189	2VEB	HIS	120	CD2	3.127584
1190	2VEB	HIS	120	ND1	4.217047
1191	2VEB	HIS	120	CG	4.266510
1192	2VEB	TRP	185	CH2	5.863505
1193	2VEB	LEU	142	CD1	6.144500
1194	2VEB	HIS	120	CB	5.683771
1195	2VEB	TRP	185	CZ3	5.261833
1196	2VEB	LEU	142	CG	6.173056
1197	2VEB	HIS	120	CA	6.386457
1198	2VEB	ILE	116	O	6.964660
1199	2VEB	HIS	120	N	6.875243
1200	2VEB	ILE	137	CB	6.983292
1201	2VEB	LEU	142	CD2	6.676723
1202	2VEB	TRP	185	CE3	6.028638
1203	2VEB	PHE	93	CG	5.963832
1205	3HX9	ALA	71	C	6.697858
1206	3HX9	HIS	75	NE2	2.161037
1207	3HX9	HIS	75	CG	4.351798

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1208	3HX9	PHE	23	CD2	9.338284
1209	3HX9	ILE	9	CG2	9.023857
1210	3HX9	HIS	75	CE1	2.959564
1211	3HX9	PHE	23	CE2	8.402145
1212	3HX9	PHE	23	CE1	8.404853
1213	3HX9	ILE	9	CB	10.034353
1214	3HX9	ASN	7	OD1	7.587216
1215	3HX9	ALA	71	O	5.763470
1216	3HX9	ASN	7	CB	9.186177
1217	3HX9	ASN	7	CA	10.695965
1218	3HX9	HIS	75	CD2	3.298557
1219	3HX9	PHE	23	CZ	7.897254
1220	3HX9	HIS	75	CB	5.820270
1221	3HX9	ILE	9	CD1	9.616978
1222	3HX9	ASN	7	CG	8.514367
1223	3HX9	PHE	23	CD1	9.357413
1224	3HX9	TRP	66	CH2	7.852796
1225	3HX9	ASN	7	ND2	9.169066
1226	3HX9	VAL	53	CG2	10.078838
1227	3HX9	VAL	53	CG1	9.844594
1228	3HX9	VAL	53	CB	10.355397
1229	3HX9	HIS	75	CA	6.621486
1230	3HX9	HIS	75	ND1	4.156833
1231	3MVF	LEU	133	CB	6.936452
1232	3MVF	LEU	123	CB	6.256287
1233	3MVF	HIS	59	NE2	2.014759
1234	3MVF	THR	121	CG2	6.595150
1235	3MVF	HIS	59	CE1	2.975441
1236	3MVF	HIS	59	CD2	3.034990
1237	3MVF	HIS	59	ND1	4.106163
1238	3MVF	HIS	59	CG	4.159371
1239	3MVF	HIS	59	CB	5.568195
1240	3MVF	LEU	133	CD2	4.998520
1241	3MVF	LEU	123	CD2	4.947831
1242	3MVF	LEU	133	CG	6.451363

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1243	3MVF	LEU	123	CD1	6.251141
1244	3MVF	LEU	123	CG	6.110708
1245	3MVF	PHE	68	CZ	5.471776
1246	3MVF	PHE	68	CE2	6.730223
1247	3MVF	PHE	68	CE1	5.542608
1248	3MVF	PHE	68	CD1	6.840606
1249	3MVF	LEU	57	CD1	6.242544
1250	3MVF	ALA	42	CB	5.827660
1252	3MVF	HIS	59	CA	6.609256
1255	3MVF	TYR	40	CD2	6.970942
1256	3MVF	LEU	133	CD1	6.980388
1257	3MVF	TYR	40	CG	6.711507
1258	3MVF	TYR	40	CB	6.595774
1259	3QZN	MET	84	CB	6.851692
1260	3QZN	MET	84	CA	6.309965
1261	3QZN	MET	84	N	5.850043
1262	3QZN	HIS	83	NE2	2.014537
1263	3QZN	HIS	83	CE1	3.007731
1264	3QZN	HIS	83	CD2	3.007864
1265	3QZN	HIS	83	ND1	4.110545
1266	3QZN	HIS	83	CG	4.142348
1267	3QZN	HIS	83	CB	5.565490
1268	3QZN	HIS	83	O	5.916970
1269	3QZN	HIS	83	C	5.814782
1270	3QZN	HIS	83	CA	6.255440
1271	3QZN	HIS	83	N	6.769288
1272	3QZN	ILE	164	CD1	6.384201
1273	3QZN	VAL	161	CG2	5.335101
1274	3QZN	VAL	161	CG1	6.990677
1275	3QZN	VAL	161	CB	6.546703
1276	3QZN	TYR	87	OH	6.350070
1277	3QZN	TYR	87	CZ	6.298706
1278	3QZN	TYR	87	CE2	5.620526
1279	3QZN	TYR	87	CD2	5.999083
1280	3QZN	TYR	87	CG	6.990261

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1281	3QZN	ILE	159	CB	5.971449
1282	3QZN	ALA	166	CB	6.907969
1283	3QZN	TYR	170	OH	4.518724
1284	3QZN	TYR	170	CZ	5.015562
1285	3QZN	TYR	170	CE2	5.062321
1286	3QZN	TYR	170	CE1	5.919869
1287	3QZN	TYR	170	CD2	5.987599
1288	3QZN	TYR	170	CD1	6.735975
1289	3QZN	TYR	170	CG	6.789363
1290	3QZN	ILE	159	CG2	5.411977
1291	3QZN	ILE	159	CG1	6.214812
1292	3QZN	HIS	168	CD2	6.973181
1293	3QZZ	LEU	142	CD2	6.810337
1294	3QZZ	LEU	142	CD1	6.509648
1295	3QZZ	LEU	142	CG	6.284455
1296	3QZZ	HIS	120	CE1	3.225914
1297	3QZZ	PHE	93	CZ	6.599510
1298	3QZZ	PHE	93	CD1	5.193243
1299	3QZZ	PHE	93	CG	6.334800
1300	3QZZ	PHE	93	CB	6.692918
1301	3QZZ	TRP	60	CZ2	6.325750
1302	3QZZ	TRP	60	CE2	6.793651
1303	3QZZ	HIS	120	ND1	4.353591
1304	3QZZ	HIS	120	CG	4.400138
1305	3QZZ	HIS	120	CA	6.485812
1306	3QZZ	TRP	185	CH2	5.787465
1307	3QZZ	HIS	120	CD2	3.256791
1308	3QZZ	ILE	137	CD1	5.400625
1309	3QZZ	ILE	137	CG2	6.903075
1310	3QZZ	ILE	116	CG2	6.274179
1311	3QZZ	ILE	116	O	6.670533
1312	3QZZ	PHE	93	CE1	5.346879
1313	3QZZ	HIS	120	N	6.981209
1314	3QZZ	HIS	120	CB	5.817278
1315	3QZZ	TRP	185	CZ3	5.529425

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1316	3QZZ	PHE	74	CZ	6.130376
1317	3QZZ	PHE	74	CE2	6.307462
1318	3QZZ	TRP	185	CZ2	6.784966
1319	3QZZ	ILE	137	CG1	6.878192
1320	3QZZ	TRP	60	NE1	6.356098
1321	3QZZ	TRP	185	CE3	6.345344
1322	3QZZ	PHE	145	CE2	5.978493
1323	3QZZ	PHE	145	CD2	5.771054
1324	3QZZ	PHE	145	CG	6.829341
1325	3QZZ	HIS	120	NE2	2.271793
1326	3QZZ	VAL	89	CG1	5.927268
1327	3SIK	ILE	131	CD1	6.481115
1328	3SIK	ALA	138	CB	6.231014
1329	3SIK	ARG	54	CG	5.962951
1330	3SIK	ARG	54	CB	6.217635
1331	3SIK	TYR	136	CZ	3.262868
1332	3SIK	TYR	136	CE1	3.949720
1333	3SIK	TYR	136	CD2	5.291753
1334	3SIK	TYR	136	CD1	5.174201
1335	3SIK	TYR	136	CG	5.768837
1336	3SIK	TYR	136	OH	2.279269
1337	3SIK	ILE	129	CD1	6.830934
1338	3SIK	ILE	129	CG2	5.924310
1339	3SIK	ILE	129	CG1	5.926524
1340	3SIK	ILE	129	CB	6.074748
1341	3SIK	TYR	140	OH	3.728919
1342	3SIK	TYR	140	CZ	4.336624
1343	3SIK	TYR	140	CE2	4.340959
1344	3SIK	TYR	140	CE1	5.403494
1345	3SIK	TYR	140	CD2	5.411071
1346	3SIK	TYR	140	CD1	6.298331
1347	3SIK	TYR	140	CG	6.321555
1348	3SIK	TYR	136	CE2	4.096641
1349	3TGC	HIS	59	NE2	2.073508
1350	3TGC	HIS	59	CE1	3.031618

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1351	3TGC	HIS	59	CD2	3.067153
1352	3TGC	HIS	59	ND1	4.143162
1353	3TGC	HIS	59	CG	4.193769
1354	3TGC	HIS	59	CB	5.605485
1355	3TGC	HIS	59	CA	6.591063
1356	3TGC	LEU	123	CD2	5.064444
1357	3TGC	LEU	123	CD1	6.334292
1358	3TGC	LEU	123	CG	6.096295
1359	3TGC	LEU	123	CB	6.139668
1360	3TGC	PHE	68	CE1	6.709550
1361	3TGC	PHE	68	CD2	6.849456
1362	3TGC	PHE	68	CZ	5.482311
1364	3TGC	THR	121	CG2	6.343084
1365	3TGC	LEU	133	CD2	4.891290
1366	3TGC	VAL	36	CG1	6.135653
1367	3TGC	LEU	133	CD1	6.995547
1368	3TGC	LEU	133	CG	6.395440
1369	3TGC	LEU	133	CB	6.978042
1372	3TGC	LEU	57	CD1	6.147624
1373	3TGC	ALA	42	CB	6.033598
1374	3TGC	TYR	40	OH	5.966614
1375	3TGC	TYR	40	CZ	6.113585
1376	3TGC	TYR	40	CE2	5.584403
1377	3TGC	TYR	40	CD2	6.204258
1378	3TGC	PHE	68	CE2	5.569867
1379	3VP5	LYS	145	CG	4.647679
1380	3VP5	LYS	145	CB	5.489262
1381	3VP5	LYS	145	O	5.884138
1382	3VP5	LYS	145	C	6.211987
1383	3VP5	LYS	145	CA	5.589317
1384	3VP5	LYS	145	N	6.702039
1385	3VP5	PHE	112	CZ	6.293359
1386	3VP5	THR	130	OG1	5.980868
1387	3VP5	THR	68	CG2	4.932643
1388	3VP5	THR	68	CB	6.459137

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1389	3VP5	HIS	72	NE2	2.117132
1390	3VP5	HIS	72	CE1	2.965993
1391	3VP5	HIS	72	CD2	3.179344
1392	3VP5	HIS	72	ND1	4.117728
1393	3VP5	HIS	72	CG	4.247640
1394	3VP5	HIS	72	CB	5.675310
1395	3VP5	HIS	72	N	6.507429
1396	3VP5	THR	68	OG1	6.984301
1397	3VP5	ILE	71	CG2	5.826383
1398	3VP5	ILE	71	C	6.987649
1399	3VP5	VAL	131	CG1	5.568423
1400	3VP5	PHE	112	CE1	6.724964
1401	3VP5	HIS	72	CA	6.165190
1402	3VP5	HIS	149	NE2	2.103609
1403	3VP5	HIS	149	CE1	2.965920
1404	3VP5	HIS	149	CD2	3.188081
1405	3VP5	TYR	91	OH	6.574739
1406	3VP5	HIS	149	ND1	4.131927
1407	3VP5	HIS	149	CG	4.260659
1408	3VP5	HIS	149	CB	5.705258
1409	3VP5	THR	68	O	6.283705
1410	3VP5	HIS	149	CA	6.173446
1411	3VP5	HIS	149	N	6.277780
1412	3VP5	VAL	148	CG1	6.781035
1413	3VP5	VAL	148	CB	6.996095
1414	3VP5	PHE	76	CE2	6.844578
1415	3VP5	LYS	145	CE	6.634337
1416	3VP5	LYS	145	CD	5.501776
1417	3ZJS	PHE	74	CZ	5.804638
1418	3ZJS	PHE	74	CE2	6.729639
1419	3ZJS	PHE	74	CE1	6.276511
1420	3ZJS	PHE	145	CE2	6.165787
1421	3ZJS	PHE	145	CD2	5.954110
1422	3ZJS	TYR	61	OH	6.548411
1423	3ZJS	PHE	93	CB	6.939455

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1424	3ZJS	HIS	120	NE2	2.059360
1425	3ZJS	HIS	120	CE1	2.908669
1426	3ZJS	HIS	120	CD2	3.168277
1427	3ZJS	HIS	120	ND1	4.083304
1428	3ZJS	HIS	120	CG	4.231957
1429	3ZJS	HIS	120	CB	5.678985
1430	3ZJS	HIS	120	CA	6.385536
1431	3ZJS	HIS	120	N	6.901157
1432	3ZJS	TRP	60	CZ2	6.391269
1433	3ZJS	TRP	60	CE2	6.655729
1434	3ZJS	TRP	60	NE1	6.053999
1435	3ZJS	TRP	185	CZ2	6.914712
1437	3ZJS	ILE	116	O	6.859685
1440	3ZJS	ILE	116	CG2	6.178215
1441	3ZJS	VAL	89	CG1	5.790982
1442	3ZJS	PHE	93	CE2	4.977692
1443	3ZJS	PHE	93	CD2	5.069659
1444	3ZJS	PHE	93	CG	6.388068
1445	3ZJS	TRP	185	CH2	5.742174
1446	3ZJS	TRP	185	CZ3	5.188422
1447	3ZJS	TRP	185	CE3	5.997883
1448	3ZJS	ILE	137	CD1	5.330212
1449	3ZJS	ILE	137	CG1	6.789524
1450	3ZJS	ILE	137	CG2	6.825342
1451	3ZJS	PHE	93	CZ	6.237529
1452	3ZJS	LEU	142	CD1	6.214702
1453	3ZJS	LEU	142	CG	6.365141
1454	4B8N	PHE	67	CZ	6.398576
1455	4B8N	PHE	67	CE1	5.206994
1456	4B8N	ILE	55	CB	6.806924
1457	4B8N	PHE	44	CD2	6.780683
1458	4B8N	PHE	67	CD1	5.207972
1459	4B8N	PHE	67	CG	6.402467
1460	4B8N	PHE	67	CB	6.873247
1461	4B8N	ILE	55	CD1	5.158658

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1462	4B8N	PHE	67	O	6.909133
1463	4B8N	ALA	54	CB	6.390793
1464	4B8N	PHE	67	CA	6.743413
1465	4B8N	HIS	71	N	6.631851
1466	4B8N	ILE	55	CG1	5.309802
1467	4B8N	LEU	70	CD1	6.337293
1468	4B8N	VAL	75	CG1	6.033658
1469	4B8N	LEU	70	CG	6.853951
1470	4B8N	GLY	51	O	6.493390
1471	4B8N	LEU	70	CB	5.993916
1472	4B8N	GLY	51	N	6.432510
1473	4B8N	GLY	50	O	6.294923
1474	4B8N	GLY	50	C	5.825586
1475	4B8N	GLY	50	CA	4.927444
1476	4B8N	GLY	50	N	4.811922
1477	4B8N	PRO	49	CD	5.624588
1478	4B8N	PRO	49	CG	6.483337
1479	4B8N	PRO	49	CB	6.381396
1480	4B8N	PRO	49	O	6.861719
1481	4B8N	LEU	70	C	6.423615
1482	4B8N	PRO	49	C	5.902910
1483	4B8N	PRO	49	CA	6.292279
1484	4B8N	PRO	49	N	5.727846
1485	4B8N	HIS	48	NE2	1.926346
1486	4B8N	HIS	48	CE1	2.862963
1487	4B8N	HIS	48	CD2	2.954577
1488	4B8N	HIS	48	ND1	4.005662
1489	4B8N	HIS	48	CG	4.078625
1490	4B8N	HIS	48	CB	5.508528
1491	4B8N	HIS	48	O	6.796537
1492	4B8N	HIS	48	C	6.100566
1493	4B8N	HIS	48	CA	6.080760
1494	4B8N	HIS	71	NE2	2.047263
1495	4B8N	HIS	71	CD2	3.054285
1496	4B8N	LEU	70	O	6.176021

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1497	4B8N	HIS	71	ND1	4.164509
1498	4B8N	HIS	71	CE1	3.025952
1499	4B8N	HIS	71	CB	5.649980
1500	4B8N	HIS	71	CA	6.538607
1501	4B8N	LEU	70	CA	6.952706
1502	4B8N	PHE	44	CZ	5.956647
1503	4B8N	HIS	71	CG	4.216480
1504	4B8N	PHE	44	CE2	5.622671
1508	4CDP	PHE	243	CZ	5.503151
1509	4CDP	PHE	243	CE2	5.205184
1510	4CDP	MET	241	CE	6.340896
1511	4CDP	PHE	243	CE1	6.874226
1512	4CDP	PHE	243	CD2	6.395301
1513	4CDP	ARG	100	NE	4.244147
1514	4CDP	HIS	193	CD2	3.093658
1515	4CDP	ARG	100	NH2	5.077263
1516	4CDP	ARG	100	NH1	6.419809
1517	4CDP	ARG	100	CZ	5.149393
1518	4CDP	ARG	100	CD	4.912842
1519	4CDP	ARG	100	CG	5.280319
1520	4CDP	ARG	100	CB	6.438838
1524	4CDP	HIS	193	NE2	2.111868
1525	4CDP	LEU	90	CD1	6.499175
1526	4CDP	HIS	193	ND1	4.215850
1527	4CDP	HIS	193	CG	4.248253
1528	4CDP	HIS	193	CB	5.657905
1529	4CDP	HIS	193	CA	6.341823
1530	4CDP	HIS	193	N	6.563416
1531	4CDP	VAL	192	CG2	5.600764
1532	4CDP	ILE	252	CD1	5.488395
1533	4CDP	HIS	193	CE1	3.108264
1534	4CDP	ILE	252	CG1	6.868024
1535	4CDP	ASP	191	OD1	6.789427
1536	4I3Q	CYS	442	C	4.698270
1537	4I3Q	CYS	442	CA	3.911617

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1538	4I3Q	MET	445	CB	6.482176
1539	4I3Q	MET	445	CA	5.997661
1540	4I3Q	MET	445	N	5.446685
1541	4I3Q	GLY	444	O	5.675947
1542	4I3Q	GLY	444	C	5.268493
1543	4I3Q	GLY	444	CA	5.138813
1544	4I3Q	GLY	444	N	4.806324
1545	4I3Q	GLY	306	N	6.469042
1546	4I3Q	PHE	435	CG	6.258619
1547	4I3Q	ILE	443	CG2	6.183244
1548	4I3Q	ILE	443	CB	6.806828
1549	4I3Q	ILE	443	C	5.918812
1550	4I3Q	ILE	443	CA	6.065666
1551	4I3Q	ILE	443	N	4.950565
1552	4I3Q	CYS	442	SG	2.075439
1553	4I3Q	CYS	442	CB	3.250313
1554	4I3Q	ARG	212	NH2	6.564614
1555	4I3Q	ARG	212	NH1	5.916129
1556	4I3Q	ARG	212	CZ	6.697803
1557	4I3Q	CYS	442	N	5.109792
1558	4I3Q	THR	309	CG2	6.233366
1559	4I3Q	THR	309	OG1	6.005998
1560	4I3Q	ASN	441	O	6.197601
1561	4I3Q	ALA	305	CA	5.838653
1562	4I3Q	THR	309	CB	6.403658
1563	4I3Q	ASN	441	C	6.080718
1564	4I3Q	GLY	306	CA	6.677164
1565	4I3Q	ALA	305	CB	5.014988
1566	4I3Q	ALA	305	O	4.814355
1567	4I3Q	ALA	305	C	5.553093
1568	4I3Q	PHE	435	CE1	5.763093
1569	4I3Q	PHE	435	CD1	5.205403
1570	4I3Q	ALA	448	CB	6.441232
1571	4I3Q	PHE	435	CB	6.263372
1572	4I3Q	PHE	435	O	6.569787

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1573	4I3Q	PHE	435	C	6.792849
1574	4I3Q	PHE	435	CA	6.278641
1575	4I3Q	PRO	434	O	6.893037
1576	4I3Q	CYS	442	O	5.469258
1577	4JET	PHE	77	CD1	5.396711
1578	4JET	PHE	77	CG	6.526201
1579	4JET	PHE	77	CB	6.711537
1580	4JET	PHE	77	O	6.850662
1581	4JET	PHE	77	C	6.647784
1582	4JET	PHE	77	CA	6.026391
1583	4JET	TYR	55	OH	6.877273
1584	4JET	PHE	77	N	6.593260
1585	4JET	TYR	75	OH	2.152890
1586	4JET	TYR	75	CZ	3.067076
1587	4JET	TYR	75	CE2	3.817746
1588	4JET	TYR	75	CE1	3.831066
1589	4JET	TYR	75	CD2	4.998270
1590	4JET	TYR	75	CD1	5.008661
1591	4JET	TYR	75	CG	5.524260
1592	4JET	TYR	75	CB	6.960877
1593	4JET	HIS	81	ND1	4.059069
1594	4JET	ILE	30	CD1	6.988601
1595	4JET	ARG	144	NH2	6.167147
1597	4JET	ARG	40	NH2	6.489466
1598	4JET	ARG	40	NH1	4.394630
1599	4JET	ARG	40	CZ	5.351691
1600	4JET	ARG	40	NE	5.456435
1601	4JET	HIS	81	NE2	5.896538
1602	4JET	ARG	40	CG	5.777773
1603	4JET	HIS	81	CD2	5.899344
1604	4JET	ARG	40	O	5.935206
1605	4JET	HIS	81	CG	4.816417
1606	4JET	HIS	81	CB	4.827998
1607	4JET	HIS	81	O	6.044402
1608	4JET	HIS	81	C	6.254399

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1609	4JET	HIS	81	CA	5.764024
1610	4JET	MET	147	CE	5.428378
1611	4JET	MET	147	SD	6.192637
1612	4JET	ARG	40	CD	4.670577
1613	4JET	HIS	81	CE1	4.868006
1614	4JET	ARG	40	CB	5.509273
1615	4JET	ARG	40	CA	6.365250
1616	4JET	PHE	50	CE1	6.875792
1617	4JET	ARG	144	NH1	5.381658
1618	4JET	ARG	144	CZ	5.964601
1619	4JET	ARG	144	NE	6.695763
1620	4JET	ARG	144	CD	6.988768
1621	4JET	PHE	77	CE1	5.734833
1622	4JET	ARG	40	C	6.653694
1623	4MF9	ARG	112	NH1	5.908430
1624	4MF9	ARG	112	CZ	4.583693
1625	4MF9	ARG	112	NE	3.954048
1626	4MF9	ARG	112	CD	4.943968
1627	4MF9	ARG	112	CG	5.215713
1628	4MF9	ARG	112	CB	6.563876
1629	4MF9	ILE	268	CD1	5.438718
1630	4MF9	ILE	268	CG1	6.746285
1631	4MF9	HIS	209	NE2	2.317556
1632	4MF9	PHE	259	CE1	6.449315
1633	4MF9	PHE	259	CZ	5.111950
1634	4MF9	PHE	259	CE2	4.954202
1635	4MF9	HIS	209	CE1	3.085814
1636	4MF9	HIS	209	CD2	3.439551
1637	4MF9	HIS	209	ND1	4.292418
1638	4MF9	HIS	209	CG	4.485889
1639	4MF9	HIS	209	CB	5.921420
1640	4MF9	HIS	209	CA	6.556937
1641	4MF9	HIS	209	N	6.752312
1642	4MF9	THR	208	OG1	6.202558
1643	4MF9	MET	257	CE	6.826627

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1644	4MF9	PHE	259	CD2	6.205870
1645	4MF9	ARG	112	NH2	4.225025
1646	4MYP	TYR	289	OH	5.731955
1647	4MYP	TYR	289	CZ	5.740930
1648	4MYP	TYR	289	CE2	4.817949
1649	4MYP	TYR	289	CE1	6.983768
1650	4MYP	TYR	289	CD2	5.412198
1651	4MYP	TYR	289	CG	6.718568
1653	4MYP	GLN	292	O	6.295350
1654	4MYP	GLN	292	C	6.800198
1655	4MYP	SER	205	OG	6.617062
1656	4MYP	SER	205	CB	6.693650
1657	4MYP	TYR	280	CG	5.557939
1659	4MYP	ALA	282	CB	6.581195
1662	4MYP	ALA	293	CB	6.207799
1663	4MYP	TYR	280	OH	2.241904
1664	4MYP	TYR	280	CZ	3.125220
1665	4MYP	TYR	280	CE2	3.638807
1666	4MYP	TYR	280	CE1	4.094491
1667	4MYP	TYR	280	CD2	4.859603
1668	4MYP	TYR	280	CD1	5.219711
1669	4MYP	GLN	292	N	6.517151
1670	4MYP	TYR	280	CB	6.984319
1671	4MYP	GLY	291	C	6.680563
1672	4MYP	GLY	291	CA	6.194217
1673	4MYP	GLY	291	N	6.999319
1674	4NL5	HIS	75	NE2	2.104978
1675	4NL5	HIS	75	CE1	3.104569
1676	4NL5	HIS	75	CD2	3.069944
1677	4NL5	HIS	75	CG	4.225192
1678	4NL5	HIS	75	CB	5.634306
1679	4NL5	HIS	75	N	6.961089
1680	4NL5	HIS	75	ND1	4.208060
1681	4NL5	ILE	9	CG1	6.173687
1682	4NL5	PHE	23	CZ	4.441792

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1683	4NL5	PHE	23	CE2	5.447105
1684	4NL5	PHE	23	CE1	4.674371
1685	4NL5	PHE	23	CD2	6.454918
1686	4NL5	PHE	23	CD1	5.826689
1687	4NL5	PHE	23	CG	6.637661
1688	4NL5	VAL	53	CG2	5.925648
1689	4NL5	ASN	7	OD1	6.317583
1690	4NL5	ASN	7	CG	5.347163
1691	4NL5	VAL	53	CB	6.117223
1692	4NL5	TRP	66	CH2	5.714910
1693	4NL5	HIS	75	CA	6.483349
1694	4NL5	ILE	9	CD1	5.340059
1695	4NL5	TRP	66	CZ3	6.561020
1696	4NL5	TRP	66	CZ2	6.429975
1697	4NL5	ASN	7	ND2	4.367008
1699	4NL5	ALA	71	O	6.805378
1701	4NL5	ASN	7	CB	5.577170
1702	4NL5	VAL	53	CG1	5.685544
1703	4UZV	PHE	119	CZ	5.563907
1704	4UZV	PHE	119	CE2	4.888108
1705	4UZV	HIS	106	CE1	2.936415
1706	4UZV	HIS	106	CD2	3.276521
1707	4UZV	HIS	106	ND1	4.133180
1708	4UZV	HIS	106	CG	4.324605
1709	4UZV	HIS	106	CB	5.784272
1710	4UZV	HIS	106	CA	6.476877
1711	4UZV	HIS	106	N	6.951515
1712	4UZV	PHE	119	CE1	6.621653
1713	4UZV	PHE	119	CD2	5.465257
1714	4UZV	PHE	119	CG	6.564430
1715	4UZV	LEU	79	CG	5.900085
1716	4UZV	ARG	105	O	6.453543
1717	4UZV	ARG	105	C	6.925435
1718	4UZV	MET	151	CB	6.579915
1719	4UZV	PHE	67	CE2	6.655780

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1720	4UZV	MET	151	SD	6.112443
1721	4UZV	MET	151	CE	5.320884
1722	4UZV	ILE	111	CD1	5.897899
1723	4UZV	LEU	102	O	6.801707
1728	4UZV	HIS	106	NE2	2.135102
1729	4UZV	PHE	67	CE1	5.827176
1730	4UZV	LEU	79	CD2	6.157220
1731	4UZV	LEU	79	CD1	6.454240
1732	4UZV	MET	151	CG	5.618995
1733	4UZV	LEU	79	CB	6.896961
1734	4UZV	PHE	53	CZ	6.997808
1735	4UZV	PHE	67	CZ	5.469994
1736	4UZV	PHE	53	CE2	6.886051
1737	4XZD	PHE	77	CB	6.624785
1738	4XZD	ARG	40	CD	5.490855
1739	4XZD	TYR	75	CG	5.396533
1740	4XZD	PHE	77	CZ	6.937227
1741	4XZD	TYR	75	CB	6.812150
1742	4XZD	PHE	77	CE1	5.566787
1743	4XZD	PHE	77	CD1	5.231466
1744	4XZD	PHE	77	CG	6.408436
1745	4XZD	PHE	77	O	6.716959
1746	4XZD	PHE	77	CA	5.941161
1747	4XZD	ARG	40	CG	5.500107
1748	4XZD	PHE	77	N	6.474273
1749	4XZD	MET	147	SD	5.934163
1750	4XZD	TYR	75	CE2	3.772469
1751	4XZD	TYR	75	CE1	3.701583
1752	4XZD	TYR	75	CD2	4.924184
1753	4XZD	TYR	75	CD1	4.866644
1754	4XZD	MET	147	CE	6.661558
1755	4XZD	ARG	40	C	6.702015
1756	4XZD	ARG	144	NH2	6.541360
1757	4XZD	ARG	144	NH1	5.250987
1758	4XZD	ARG	144	CZ	6.101746

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1759	4XZD	ARG	144	NE	6.838649
1760	4XZD	ARG	40	NE	6.060155
1761	4XZD	ARG	144	CD	6.945827
1762	4XZD	PHE	77	C	6.580665
1763	4XZD	HIS	81	CE1	4.673183
1764	4XZD	TYR	55	OH	6.821652
1765	4XZD	ARG	40	O	5.976479
1766	4XZD	TYR	75	OH	2.157519
1767	4XZD	ARG	40	NH1	4.694000
1768	4XZD	ARG	40	CZ	5.729084
1769	4XZD	THR	82	N	6.830323
1770	4XZD	HIS	81	NE2	5.692255
1771	4XZD	TYR	75	CZ	3.008552
1772	4XZD	ARG	40	CB	5.579011
1773	4XZD	HIS	81	ND1	3.821248
1774	4XZD	HIS	81	CG	4.565995
1775	4XZD	ARG	40	CA	6.464511
1776	4XZD	HIS	81	CB	4.599501
1777	4XZD	HIS	81	O	5.665049
1778	4XZD	HIS	81	C	5.860481
1779	4XZD	HIS	81	CA	5.409693
1780	4XZD	HIS	81	N	6.673948
1781	4XZD	HIS	81	CD2	5.669724
1782	4XZD	ARG	40	NH2	6.725728
1783	4Y1Q	ARG	40	C	6.665410
1784	4Y1Q	ARG	40	CA	6.429167
1785	4Y1Q	MET	147	CE	5.679400
1786	4Y1Q	PHE	77	CE1	6.104351
1787	4Y1Q	PHE	77	CD1	5.877343
1788	4Y1Q	HIS	81	ND1	5.426768
1789	4Y1Q	PHE	77	C	6.923090
1790	4Y1Q	PHE	77	CA	6.390460
1791	4Y1Q	PHE	77	N	6.768987
1792	4Y1Q	ARG	144	NH2	6.770579
1793	4Y1Q	ALA	75	CB	6.722226

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1794	4Y1Q	ARG	144	NH1	5.258854
1795	4Y1Q	HIS	81	NE2	4.913699
1796	4Y1Q	PHE	50	CE1	6.381295
1797	4Y1Q	MET	147	SD	6.552120
1798	4Y1Q	ARG	144	CZ	6.232237
1799	4Y1Q	PHE	50	CD1	6.730337
1800	4Y1Q	ARG	40	CZ	5.467761
1801	4Y1Q	ARG	40	NE	5.728993
1802	4Y1Q	HIS	81	CD2	4.049749
1803	4Y1Q	ARG	40	CD	5.070919
1804	4Y1Q	ARG	144	CD	6.916519
1805	4Y1Q	ARG	40	NH2	6.530842
1806	4Y1Q	HIS	81	CE1	5.656618
1807	4Y1Q	ARG	40	NH1	4.412558
1808	4Y1Q	TYR	55	OH	6.699820
1809	4Y1Q	HIS	81	CG	4.442063
1810	4Y1Q	HIS	81	CB	4.506902
1811	4Y1Q	HIS	81	O	5.582811
1812	4Y1Q	HIS	81	C	5.991993
1813	4Y1Q	HIS	81	CA	5.562055
1814	4Y1Q	HIS	81	N	6.810231
1815	4Y1Q	ARG	40	CG	5.558394
1816	4Y1Q	ARG	40	CB	5.504676
1817	4Y1Q	ARG	144	NE	6.951212
1818	4Y1Q	ARG	40	O	5.883335
1819	5CN5	HIS	97	NE2	5.499594
1820	5CN5	HIS	97	CD2	5.005579
1821	5CN5	HIS	97	ND1	6.673470
1822	5CN5	HIS	97	CG	5.838143
1823	5CN5	HIS	97	CB	6.296036
1824	5CN5	VAL	68	CG2	4.630775
1825	5CN5	VAL	68	CB	5.712726
1826	5CN5	VAL	68	CA	6.265042
1827	5CN5	HIS	93	CD2	3.277478
1828	5CN5	VAL	68	CG1	5.617449

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1830	5CN5	HIS	93	NE2	2.229233
1831	5CN5	HIS	97	CE1	6.485629
1832	5CN5	HIS	93	CE1	3.115222
1833	5CN5	HIS	93	ND1	4.267690
1834	5CN5	HIS	93	CG	4.375619
1835	5CN5	HIS	93	CB	5.799797
1836	5CN5	HIS	93	CA	6.543046
1837	5CN5	HIS	93	N	6.994836
1838	5CN5	SER	92	OG	6.529632
1839	5CN5	HIS	64	CD2	5.654299
1840	5CN5	HIS	64	ND1	6.583463
1841	5CN5	HIS	64	CG	6.764052
1842	5CN5	PHE	43	CZ	5.374377
1843	5CN5	HIS	64	NE2	4.650697
1844	5CN5	PHE	43	CE2	5.429861
1845	5CN5	PHE	43	CE1	6.508868
1846	5CN5	PHE	43	CD2	6.611682
1847	5CN5	LEU	104	CD2	6.517400
1848	5CN5	HIS	64	CE1	5.371125
1849	5CN5	LEU	89	CD2	6.061927
1850	5CN5	LEU	89	CD1	6.858400
1851	5CN5	LEU	89	O	6.902204
1852	5CN5	ILE	107	CD1	6.767432
1853	5CN5	ILE	99	CD1	6.420675
1854	5CN5	ILE	99	CG2	6.718646
1855	5CN5	ILE	99	CG1	5.812304
1856	5CN5	ILE	99	CB	6.689823
1858	5GJ3	ARG	142	NH1	8.179276
1859	5GJ3	ARG	142	CZ	8.778676
1860	5GJ3	ARG	142	NE	8.979885
1861	5GJ3	ARG	142	CD	8.607854
1862	5GJ3	ARG	142	CG	9.355975
1863	5GJ3	ARG	142	CB	9.765637
1864	5GJ3	GLN	141	NE2	8.788580
1865	5GJ3	GLN	141	OE1	11.054586

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1866	5GJ3	GLN	141	CD	9.936146
1867	5GJ3	ARG	241	CZ	5.277230
1868	5GJ3	GLN	141	CG	9.984684
1869	5GJ3	ARG	241	NH2	4.474480
1870	5GJ3	TYR	140	OH	6.129911
1871	5GJ3	TYR	140	CZ	6.603546
1872	5GJ3	ARG	241	CG	6.052647
1873	5GJ3	TYR	239	OH	2.057052
1874	5GJ3	TYR	140	CE1	7.188333
1875	5GJ3	TYR	140	CD2	7.736499
1876	5GJ3	TYR	140	CD1	7.968897
1877	5GJ3	TYR	140	CG	8.235358
1878	5GJ3	TYR	140	CB	9.404934
1879	5GJ3	ARG	241	CD	4.883389
1880	5GJ3	TYR	239	CZ	3.129005
1881	5GJ3	TYR	239	CE2	4.244972
1882	5GJ3	ARG	241	CB	6.400599
1883	5GJ3	TYR	239	CD2	5.423697
1884	5GJ3	SER	124	OG	10.773736
1885	5GJ3	TYR	239	CG	5.741268
1886	5GJ3	ARG	241	NE	5.431109
1887	5GJ3	TYR	239	CE1	3.629462
1888	5GJ3	ARG	241	NH1	6.278162
1889	5GJ3	TYR	239	CD1	4.966826
1890	5GJ3	SER	124	CB	9.703852
1891	5GJ3	ARG	142	NH2	9.446755
1892	5GJ3	TYR	140	CE2	6.893562
1893	5KZL	HIS	15	ND1	4.362024
1894	5KZL	GLY	128	O	4.717154
1895	5KZL	HIS	15	CG	4.371613
1896	5KZL	GLY	128	C	5.112458
1897	5KZL	HIS	15	CB	5.789015
1898	5KZL	GLY	128	CA	4.693838
1899	5KZL	HIS	15	O	6.681930
1900	5KZL	GLY	128	N	6.000414

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1901	5KZL	HIS	15	C	6.913432
1902	5KZL	HIS	15	NE2	2.263741
1903	5KZL	HIS	15	CA	6.513236
1904	5KZL	VAL	124	O	6.607237
1905	5KZL	PHE	195	CZ	6.490501
1906	5KZL	GLU	19	OE2	5.803913
1907	5KZL	PHE	195	CE1	6.211680
1908	5KZL	LEU	127	O	6.670104
1909	5KZL	LEU	127	C	6.793273
1910	5KZL	LEU	136	CD1	6.422701
1911	5KZL	GLY	132	CA	5.718532
1912	5KZL	GLY	132	N	5.691592
1913	5KZL	SER	131	OG	6.605168
1914	5KZL	SER	131	CB	5.777476
1915	5KZL	SER	131	O	6.902050
1916	5KZL	SER	131	C	6.282734
1917	5KZL	SER	131	CA	6.625728
1918	5KZL	HIS	15	CE1	3.221258
1919	5KZL	HIS	15	CD2	3.260597
1920	5KZL	ASP	129	N	6.318347
1921	5O1L	GLU	148	CG	6.396575
1922	5O1L	ILE	227	CG1	6.973430
1923	5O1L	VAL	152	CG2	6.293389
1925	5O1L	VAL	197	CG1	6.392188
1930	5O1L	HIS	198	CE1	2.960033
1931	5O1L	HIS	198	CD2	3.058523
1932	5O1L	HIS	198	ND1	4.119976
1933	5O1L	HIS	198	CG	4.179972
1934	5O1L	HIS	198	CA	6.135598
1935	5O1L	HIS	198	N	6.367407
1936	5O1L	VAL	197	CB	6.904140
1937	5O1L	ILE	222	CD1	5.454421
1938	5O1L	ILE	222	CB	6.700079
1939	5O1L	LEU	171	CD2	5.871784
1940	5O1L	LEU	171	CG	6.157864

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1941	5O1L	HIS	198	NE2	2.008409
1942	5O1L	ILE	222	CG2	5.717054
1943	5O1L	ILE	222	CG1	6.228249
1944	5O1L	THR	194	CG2	4.863475
1945	5O1L	THR	194	OG1	6.732273
1946	5O1L	THR	194	CB	6.310660
1947	5O1L	THR	194	O	6.209525
1948	5O1L	THR	194	C	6.855242
1949	5O1L	THR	194	CA	6.862712
1950	5O1L	THR	230	CG2	6.574103
1951	5O1L	HIS	198	CB	5.613320
1952	5O1L	GLU	148	OE2	6.340688
1953	5O1L	LEU	171	CD1	5.199565
1954	5O1L	GLU	148	CD	6.584651
1955	5O1M	THR	230	OG1	6.704437
1956	5O1M	THR	168	CB	6.716431
1957	5O1M	HIS	198	ND1	4.228786
1958	5O1M	HIS	198	CG	4.285748
1959	5O1M	THR	168	CA	6.786040
1960	5O1M	THR	168	N	6.597112
1961	5O1M	LYS	167	NZ	2.394322
1962	5O1M	LYS	167	CE	3.425470
1963	5O1M	HIS	198	CD2	3.148354
1964	5O1M	HIS	198	N	6.358799
1965	5O1M	VAL	152	CG2	6.250877
1966	5O1M	LYS	167	CG	4.772075
1967	5O1M	VAL	197	CB	6.924162
1968	5O1M	ILE	222	CG2	5.991532
1969	5O1M	LYS	167	C	6.677968
1970	5O1M	LYS	167	CA	6.982216
1971	5O1M	HIS	198	CB	5.708988
1972	5O1M	THR	194	CG2	5.053058
1973	5O1M	THR	194	OG1	6.976250
1974	5O1M	THR	194	CB	6.495937
1975	5O1M	THR	194	O	6.143256

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1976	5O1M	THR	194	C	6.825779
1977	5O1M	THR	194	CA	6.965214
1978	5O1M	HIS	198	CA	6.167626
1979	5O1M	THR	230	CG2	6.503399
1980	5O1M	LYS	167	CD	4.069773
1981	5O1M	VAL	197	CG1	6.337990
1982	5O1M	THR	168	CG2	5.394286
1983	5O1M	ILE	222	CD1	5.544717
1984	5O1M	LYS	167	CB	5.830588
1985	5O1M	LYS	167	O	6.853283
1986	5O1M	ILE	222	CG1	6.462420
1987	5O1M	ILE	222	CB	6.965598
1988	5O1M	HIS	198	NE2	2.143583
1989	5O1M	HIS	198	CE1	3.099839
1990	5VEU	PHE	434	C	6.660407
1991	5VEU	GLY	443	N	5.092847
1992	5VEU	THR	309	OG1	5.879926
1993	5VEU	ILE	442	CG2	6.410294
1994	5VEU	PHE	434	CE1	5.718749
1995	5VEU	PHE	434	CD1	5.205940
1996	5VEU	ALA	447	CB	6.667315
1997	5VEU	PHE	434	CB	6.245330
1998	5VEU	PHE	434	CA	6.234979
1999	5VEU	VAL	369	CG2	6.886497
2001	5VEU	ASN	440	O	6.478484
2003	5VEU	ALA	305	CA	6.262435
2004	5VEU	ALA	305	C	6.764115
2006	5VEU	MET	444	N	5.803810
2007	5VEU	PHE	434	O	6.308836
2008	5VEU	GLY	443	C	5.543658
2009	5VEU	GLY	443	CA	5.543488
2012	5VEU	MET	444	CB	6.762190
2016	5VEU	ILE	442	CB	6.813521
2017	5VEU	ILE	442	C	6.140402
2018	5VEU	ILE	442	CA	6.175203

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
2019	5VEU	ILE	442	N	5.058254
2020	5VEU	CYS	441	O	5.807369
2022	5VEU	MET	444	CA	6.289599
2023	5VEU	ALA	305	O	6.691834
2024	5VEU	CYS	441	CB	3.500679
2025	5VEU	CYS	441	C	4.956818
2026	5VEU	CYS	441	CA	4.203011
2027	5VEU	GLY	443	O	5.751295
2028	5VEU	PHE	434	CG	6.214903
2029	5VEU	ALA	305	CB	5.160255
2032	5VEU	ASN	440	C	6.339241
2033	5VEU	THR	309	CG2	5.668263
2034	5VEU	PRO	433	O	6.574196
2036	5VEU	CYS	441	N	5.380733
2037	5VEU	CYS	441	SG	2.248175
2038	5VEU	THR	309	CB	6.139336
2039	6A2J	ALA	259	CA	6.937825
2040	6A2J	VAL	182	CG2	6.605901
2041	6A2J	ALA	220	CB	5.986896
2042	6A2J	VAL	182	CB	6.753078
2043	6A2J	GLY	179	N	5.777355
2044	6A2J	HIS	216	CG	4.226515
2045	6A2J	THR	178	OG1	6.735056
2046	6A2J	GLY	179	C	5.733550
2047	6A2J	GLY	179	CA	4.779391
2048	6A2J	HIS	216	ND1	4.184094
2049	6A2J	ARG	217	N	6.781589
2050	6A2J	HIS	216	NE2	2.092798
2051	6A2J	HIS	216	CE1	3.068636
2052	6A2J	GLY	262	C	6.042717
2053	6A2J	HIS	216	CD2	3.087929
2054	6A2J	THR	178	O	6.870559
2055	6A2J	THR	178	C	6.710930
2056	6A2J	ILE	265	CD1	5.663965
2057	6A2J	ILE	265	CG1	6.879688

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
2058	6A2J	HIS	216	CB	5.641654
2059	6A2J	ALA	180	N	6.687029
2060	6A2J	HIS	216	C	6.355372
2061	6A2J	GLY	262	O	6.206764
2062	6A2J	HIS	216	CA	6.587911
2063	6A2J	GLY	262	N	5.991880
2064	6A2J	VAL	175	O	6.183640
2065	6A2J	SER	261	C	6.949581
2066	6A2J	GLY	262	CA	5.042220
2067	6A2J	HIS	278	NE2	2.097124
2068	6A2J	HIS	278	CE1	3.084577
2069	6A2J	HIS	278	CD2	3.076644
2070	6A2J	HIS	278	ND1	4.195480
2071	6A2J	HIS	278	CG	4.225202
2072	6A2J	HIS	278	CB	5.639445
2073	6A2J	HIS	278	O	6.179156
2074	6A2J	HIS	278	C	6.775178
2075	6A2J	HIS	278	CA	6.627579
2076	6A2J	HIS	216	O	6.170588
2077	6A2J	GLN	258	NE2	4.668084
2078	6A2J	GLN	258	OE1	6.633805
2079	6A2J	GLN	258	CD	5.618422
2080	6A2J	GLN	258	CG	5.742837
2081	6A2J	GLN	258	O	5.679824
2082	6A2J	GLN	258	C	6.479023
2083	6A2J	VAL	175	CG1	6.221186
2084	6A2J	GLY	179	O	5.904093
2085	7C74	ARG	348	NH1	6.634371
2086	7C74	ARG	348	CZ	6.877092
2087	7C74	ARG	348	NE	6.575349
2088	7C74	ARG	348	CD	5.975483
2089	7C74	ARG	348	CG	5.217041
2090	7C74	ARG	348	CB	5.945434
2091	7C74	ARG	348	O	6.372874
2092	7C74	ARG	348	N	6.760186

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
2093	7C74	HIS	109	CG	6.997955
2094	7C74	ASP	108	OD2	5.766923
2095	7C74	ASP	108	OD1	5.834435
2096	7C74	ASP	108	CG	5.892897
2097	7C74	ASP	108	CB	6.575347
2098	7C74	PHE	347	O	6.478230
2099	7C74	GLN	105	NE2	4.682805
2100	7C74	GLN	105	OE1	6.559310
2101	7C74	GLN	105	CD	5.387245
2102	7C74	GLN	105	CG	5.030685
2103	7C74	GLN	105	CB	5.976391
2104	7C74	HIS	109	CE1	5.947116
2105	7C74	GLN	105	CA	6.366871
2106	7C74	ASN	437	ND2	6.428557
2107	7C74	ASN	437	OD1	6.552144
2108	7C74	ASN	437	CG	6.979473
2109	7C74	HIS	109	CD2	5.815061
2110	7C74	GLU	258	OE2	5.841099
2111	7C74	GLU	258	OE1	6.188822
2112	7C74	GLU	258	CD	6.133430
2113	7C74	GLU	258	CG	6.870976
2114	7C74	HIS	351	NE2	2.443762
2115	7C74	HIS	351	CE1	3.562735
2116	7C74	HIS	351	CD2	3.209429
2117	7C74	ARG	348	C	6.561018
2118	7C74	HIS	351	CG	4.430495
2119	7C74	HIS	351	CB	5.763234
2120	7C74	HIS	351	CA	6.034276
2121	7C74	HIS	351	N	5.934872
2122	7C74	ARG	348	CA	5.823940
2123	7C74	HIS	109	NE2	5.050670
2124	7C74	GLY	350	C	6.439792
2125	7C74	GLY	350	CA	6.535492
2126	7C74	GLY	350	N	6.844489
2127	7C74	LEU	433	CD2	5.037286

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
2128	7C74	LEU	433	CD1	5.077063
2129	7C74	LEU	433	CG	5.712261
2130	7C74	HIS	351	ND1	4.574630
2131	7DMR	ARG	348	NE	6.408627
2132	7DMR	ARG	348	CG	5.295503
2133	7DMR	ASN	437	CG	6.914300
2134	7DMR	HIS	351	NE2	2.009632
2135	7DMR	ARG	348	O	6.454607
2136	7DMR	HIS	351	CD2	3.026161
2137	7DMR	HIS	351	CA	5.928909
2138	7DMR	GLY	350	O	6.903837
2139	7DMR	GLY	350	C	6.376621
2140	7DMR	GLY	350	CA	6.803395
2141	7DMR	ARG	348	NH1	6.674281
2142	7DMR	LEU	433	CD2	4.667452
2143	7DMR	LEU	433	CD1	5.416929
2144	7DMR	ARG	348	CD	5.921899
2145	7DMR	ASP	108	OD2	6.081939
2146	7DMR	HIS	351	ND1	4.107251
2147	7DMR	HIS	109	NE2	5.135479
2148	7DMR	ASP	108	CG	6.137863
2149	7DMR	ASP	108	CB	6.743120
2150	7DMR	ARG	348	CA	5.825545
2151	7DMR	ARG	348	N	6.752036
2152	7DMR	ASN	437	ND2	6.613466
2153	7DMR	HIS	109	CE1	5.991157
2154	7DMR	ARG	348	CB	5.823186
2155	7DMR	GLU	258	CD	6.270833
2156	7DMR	ARG	348	C	6.621339
2157	7DMR	GLU	258	OE2	6.165783
2158	7DMR	PHE	347	O	6.671472
2159	7DMR	HIS	109	CD2	5.971041
2161	7DMR	GLN	105	NE2	4.411977
2162	7DMR	HIS	351	CG	4.145017
2163	7DMR	GLN	105	OE1	6.213353

Table B.9: HEM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
2164	7DMR	GLN	105	CG	5.072883
2165	7DMR	GLN	105	CB	5.884637
2166	7DMR	HIS	351	CE1	2.988168
2167	7DMR	GLN	105	CA	6.346229
2168	7DMR	HIS	351	N	5.854069
2169	7DMR	GLU	258	OE1	6.080170
2170	7DMR	ASP	108	OD1	6.101163
2171	7DMR	ASN	437	OD1	6.246283
2172	7DMR	GLN	105	CD	5.174413
2173	7DMR	ARG	348	CZ	6.732562
2174	7DMR	LEU	433	CG	5.591102
2175	7DMR	HIS	351	CB	5.553912

Table B.10: HEC: All Distances, Atoms to Fe

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1	1BBH	TYR	16	CG	3.768724
2	1BBH	TYR	16	CB	4.351793
3	1BBH	TYR	16	O	6.032159
4	1BBH	TYR	16	C	6.047776
5	1BBH	TYR	16	CA	5.394955
6	1BBH	TYR	16	N	6.524640
7	1BBH	CYS	121	CB	5.578638
8	1BBH	CYS	121	O	5.125611
9	1BBH	CYS	121	CA	5.746306
10	1BBH	CYS	124	C	6.560352
11	1BBH	ARG	129	NH2	4.657992
12	1BBH	ARG	129	NH1	6.305764
13	1BBH	ARG	129	CZ	5.340426
14	1BBH	ARG	129	NE	5.207341
15	1BBH	ARG	129	CD	6.312478

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
16	1BBH	TYR	58	OH	6.554347
17	1BBH	ARG	129	CB	6.340612
18	1BBH	CYS	121	SG	6.411919
19	1BBH	CYS	121	C	5.823307
20	1BBH	MET	19	CE	6.049470
21	1BBH	HIS	125	NE2	2.019389
22	1BBH	HIS	125	CE1	2.978473
23	1BBH	HIS	125	CD2	3.006544
24	1BBH	HIS	125	ND1	4.113194
25	1BBH	HIS	125	CG	4.164334
26	1BBH	HIS	125	CB	5.581871
27	1BBH	HIS	125	CA	5.932117
28	1BBH	CYS	124	SG	6.078930
29	1BBH	CYS	124	CB	6.176895
30	1BBH	HIS	125	N	5.955199
31	1BBH	GLU	17	N	6.940695
32	1BBH	TYR	16	OH	5.099061
33	1BBH	TYR	16	CZ	4.254561
34	1BBH	TYR	16	CE2	4.463795
35	1BBH	TYR	16	CE1	3.833128
36	1BBH	TYR	16	CD2	4.234962
37	1BBH	TYR	16	CD1	3.540375
38	1BBH	ARG	129	CG	6.371042
39	1S56	TYR	33	OH	5.480355
40	1S56	MET	77	O	6.944303
43	1S56	HIS	81	CA	6.483579
44	1S56	ILE	86	CD1	5.878780
45	1S56	PHE	46	CZ	5.412014
46	1S56	PHE	46	CE2	6.736095
47	1S56	PHE	46	CE1	5.200905
48	1S56	PHE	46	CD1	6.404458
49	1S56	VAL	80	CG2	5.585206
50	1S56	VAL	126	CG2	5.994128
51	1S56	GLN	58	NE2	4.758584
52	1S56	GLN	58	OE1	6.404068

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
53	1S56	VAL	126	CG1	5.591172
54	1S56	GLN	58	CD	5.918043
55	1S56	GLN	58	CG	6.942411
56	1S56	VAL	80	CB	6.460712
57	1S56	VAL	126	CB	6.503475
58	1S56	VAL	80	C	6.893701
59	1S56	VAL	94	CG1	6.626107
60	1S56	HIS	81	NE2	2.136891
61	1S56	HIS	81	CE1	3.056065
62	1S56	HIS	81	CD2	3.179857
63	1S56	HIS	81	ND1	4.203043
64	1S56	HIS	81	CG	4.293691
65	1S56	HIS	81	CB	5.728508
67	1S56	LEU	54	CD2	5.985464
68	1S56	LEU	54	CD1	5.470210
69	1S56	HIS	81	N	6.718588
70	1S56	LEU	54	CG	6.386831
71	1S56	VAL	80	CG1	5.884109
72	1S56	TYR	33	CZ	6.589193
73	1S56	TYR	33	CE1	6.686496
74	1S56	MET	77	CE	5.896541
75	1S56	MET	77	SD	5.722004
76	1W2L	CYS	18	O	6.272480
77	1W2L	HIS	22	CE1	2.952828
78	1W2L	MET	76	CE	3.331224
79	1W2L	MET	76	SD	2.275594
80	1W2L	MET	76	CG	3.407807
81	1W2L	MET	76	CB	4.680531
82	1W2L	MET	76	C	6.161429
83	1W2L	VAL	75	C	6.694753
84	1W2L	HIS	22	CG	4.165408
85	1W2L	HIS	22	NE2	2.019935
86	1W2L	ILE	61	CA	6.955555
87	1W2L	HIS	22	CD2	3.043257
88	1W2L	HIS	22	ND1	4.110576

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
89	1W2L	SER	60	CB	6.743385
90	1W2L	HIS	22	CB	5.583109
91	1W2L	SER	60	C	6.654549
92	1W2L	SER	60	O	6.014503
93	1W2L	HIS	22	CA	6.535062
94	1W2L	PRO	77	N	6.185218
95	1W2L	HIS	22	N	6.395979
96	1W2L	CYS	21	SG	6.487459
97	1W2L	CYS	21	CB	5.467826
98	1W2L	CYS	21	O	6.325560
99	1W2L	CYS	21	CA	6.553338
100	1W2L	MET	76	CA	5.067215
101	1W2L	CYS	18	CA	6.391381
102	1W2L	MET	76	N	5.901524
103	1W2L	PRO	32	CD	5.998967
104	1W2L	PRO	32	CG	6.506187
105	1W2L	PRO	32	O	6.656122
106	1W2L	CYS	18	SG	6.839096
107	1W2L	CYS	18	CB	6.394080
108	1W2L	PRO	32	N	6.669496
109	1W2L	PHE	34	CZ	5.340171
110	1W2L	CYS	18	C	6.877490
111	1W2L	GLY	31	C	6.810943
112	1W2L	GLY	31	CA	6.076145
113	1W2L	GLY	31	N	6.810543
114	1W2L	PHE	34	CE2	6.565580
115	1W2L	PRO	77	CD	5.434386
116	1W2L	PHE	34	CE1	5.318068
117	1W2L	PRO	77	CG	6.595929
118	1W2L	VAL	75	O	6.812888
119	1W2L	CYS	21	C	6.283770
120	1W2L	TYR	80	OH	6.673428
121	1W2L	TYR	80	CZ	6.636632
122	1W2L	TYR	80	CE2	5.644992
123	1W2L	TYR	80	CD2	6.044178

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
124	1W2L	PHE	34	CD1	6.518920
125	1W2L	ILE	61	CG1	6.723535
126	2BC5	LEU	10	CD1	5.360121
127	2BC5	LEU	10	CG	6.600328
128	2BC5	LEU	10	CB	6.501825
129	2BC5	ARG	106	CB	6.430360
130	2BC5	CYS	98	CA	5.637823
131	2BC5	MET	7	O	5.990477
132	2BC5	MET	7	CA	5.165634
133	2BC5	MET	7	N	6.214714
134	2BC5	HIS	102	CE1	3.116663
135	2BC5	HIS	102	CD2	2.899208
136	2BC5	HIS	102	ND1	4.164600
137	2BC5	HIS	102	CG	4.097269
138	2BC5	HIS	102	CB	5.487557
139	2BC5	HIS	102	CA	5.858937
140	2BC5	MET	7	CE	3.536180
141	2BC5	MET	7	SD	2.358383
142	2BC5	HIS	102	N	5.844368
143	2BC5	CYS	101	SG	6.042141
144	2BC5	MET	7	CG	3.612198
145	2BC5	ARG	106	NH2	6.317759
146	2BC5	LEU	3	CD1	6.557423
147	2BC5	MET	7	CB	4.392171
148	2BC5	CYS	101	CA	6.960467
149	2BC5	CYS	101	CB	6.016649
150	2BC5	ASN	99	N	6.936196
151	2BC5	CYS	98	SG	6.531669
152	2BC5	ARG	106	CG	6.496541
153	2BC5	CYS	98	O	5.191848
154	2BC5	CYS	98	CB	5.609865
155	2BC5	CYS	98	C	5.789260
156	2BC5	LEU	3	CG	6.801442
157	2BC5	CYS	98	N	6.983490
158	2BC5	LEU	3	O	6.869998

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
159	2BC5	ARG	106	NH1	4.997419
160	2BC5	MET	7	C	6.025465
161	2BC5	CYS	101	C	6.559805
162	2BC5	PHE	65	CZ	6.206137
163	2BC5	PHE	65	CE2	6.197666
164	2BC5	ARG	106	CZ	5.493429
165	2BC5	ARG	106	NE	5.524917
166	2BC5	ARG	106	CD	6.469516
167	2BC5	HIS	102	NE2	2.026659
168	2BH5	TYR	79	CD2	6.106726
169	2BH5	PHE	102	CG	6.993689
170	2BH5	PHE	102	CB	6.460544
171	2BH5	PHE	102	O	6.867527
172	2BH5	LEU	39	CD2	5.741572
173	2BH5	LEU	39	CD1	5.397242
174	2BH5	LEU	39	CG	6.047540
175	2BH5	CYS	15	CB	6.273959
176	2BH5	LYS	100	CE	3.042296
177	2BH5	LYS	100	CD	3.607500
178	2BH5	LYS	100	CA	6.970077
179	2BH5	PRO	37	CG	6.313316
180	2BH5	PRO	37	O	6.469326
181	2BH5	PRO	37	N	6.305872
182	2BH5	VAL	80	CG1	6.887770
183	2BH5	GLY	36	C	6.335983
184	2BH5	GLY	36	CA	5.611445
185	2BH5	GLY	36	N	6.430717
186	2BH5	LYS	100	NZ	1.893983
187	2BH5	PHE	102	CD2	6.622745
188	2BH5	HIS	19	NE2	1.936381
189	2BH5	HIS	19	CE1	2.876087
190	2BH5	HIS	19	CD2	2.985557
191	2BH5	HIS	19	ND1	4.006787
192	2BH5	HIS	19	CG	4.089234
193	2BH5	HIS	19	CB	5.514117

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
194	2BH5	HIS	19	CA	6.462897
195	2BH5	CYS	18	SG	6.561520
196	2BH5	CYS	18	CB	5.640711
197	2BH5	CYS	18	O	6.526211
198	2BH5	CYS	18	C	6.403953
199	2BH5	CYS	18	CA	6.713588
200	2BH5	LYS	100	CG	4.911215
201	2BH5	TYR	79	OH	5.222750
202	2BH5	LYS	100	CB	5.457412
203	2BH5	CYS	15	SG	6.744431
204	2BH5	HIS	19	N	6.399261
205	2BH5	CYS	15	O	6.140470
206	2BH5	CYS	15	C	6.863968
207	2BH5	CYS	15	CA	6.544715
208	2BH5	PRO	83	CG	6.953188
209	2BH5	PRO	37	CD	5.721633
210	2BH5	TYR	79	CZ	5.692009
211	2BH5	TYR	79	CE2	5.119377
214	3EAH	TRP	144	CZ2	5.897099
216	3EAH	TRP	144	CE2	5.510177
217	3EAH	TRP	144	NE1	4.665090
218	3EAH	TRP	144	CD2	6.411670
219	3EAH	TRP	144	CD1	5.179002
220	3EAH	TRP	144	CG	6.224027
226	3EAH	ARG	153	CG	6.371859
228	3EAH	PHE	319	CE1	5.984587
229	3EAH	ARG	153	CA	6.956565
230	3EAH	CYS	150	CB	3.252402
231	3EAH	ARG	153	N	6.215203
232	3EAH	GLY	152	O	6.170630
233	3EAH	GLY	152	CA	5.467468
234	3EAH	GLY	152	N	5.042421
235	3EAH	GLY	152	C	5.828338
236	3EAH	VAL	151	CG1	6.226488
237	3EAH	VAL	151	CB	6.873725

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
239	3EAH	VAL	151	C	6.134121
240	3EAH	VAL	151	CA	6.217950
241	3EAH	VAL	151	N	5.067435
242	3EAH	CYS	150	SG	2.366787
243	3EAH	TRP	322	O	6.529256
244	3EAH	CYS	150	O	5.770370
245	3EAH	CYS	150	C	4.908984
246	3EAH	CYS	150	CA	4.045023
247	3EAH	CYS	150	N	5.140972
248	3EAH	PHE	319	CD1	6.290067
250	3EAH	ARG	149	O	5.760264
251	3EAH	ARG	149	C	5.846364
253	3EAH	ALA	147	CB	6.240842
254	3X15	PRO	25	O	6.636546
255	3X15	PRO	25	N	6.479568
256	3X15	GLY	24	C	6.579861
257	3X15	GLY	24	CA	5.838155
258	3X15	GLY	24	N	6.638694
259	3X15	HIS	16	CA	6.534752
260	3X15	CYS	15	SG	6.403522
261	3X15	CYS	15	O	5.850242
262	3X15	HIS	16	CG	4.160431
263	3X15	CYS	15	CA	6.400988
264	3X15	PHE	44	CZ	6.164195
265	3X15	ILE	30	CD1	5.838773
266	3X15	PRO	25	CD	5.714118
267	3X15	HIS	16	CD2	3.036362
268	3X15	PHE	44	CE2	5.884471
269	3X15	HIS	16	NE2	2.034065
270	3X15	HIS	16	CB	5.578454
271	3X15	HIS	16	N	6.429374
272	3X15	HIS	16	CE1	3.000765
273	3X15	CYS	15	CB	5.423303
274	3X15	CYS	15	C	6.071855
275	3X15	CYS	15	N	6.923760

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
276	3X15	ILE	30	CG1	6.986917
277	3X15	HIS	16	ND1	4.110256
278	3X15	CYS	12	SG	6.833584
279	3X15	CYS	12	CB	6.404249
280	3X15	CYS	12	O	5.833958
281	3X15	CYS	12	C	6.668691
282	3X15	CYS	12	CA	6.517488
283	3X15	PRO	25	CG	6.181197
284	5KPF	TYR	67	OH	4.782875
285	5KPF	PRO	71	CG	6.976183
286	5KPF	PHE	82	CD1	6.786896
287	5KPF	PHE	82	CG	6.214998
288	5KPF	PHE	82	CB	5.779976
289	5KPF	CYS	14	CB	6.411157
290	5KPF	HIS	18	NE2	1.983810
291	5KPF	TYR	67	CE2	5.484460
292	5KPF	LEU	32	CD2	6.023553
293	5KPF	LEU	32	CD1	5.964605
294	5KPF	LEU	32	CG	6.446949
295	5KPF	HIS	18	CE1	2.938552
296	5KPF	HIS	18	CD2	3.000836
297	5KPF	MET	80	CE	3.397915
298	5KPF	MET	80	SD	2.297111
299	5KPF	MET	80	CG	3.417184
300	5KPF	MET	80	CB	4.198483
301	5KPF	MET	80	O	6.571530
302	5KPF	ALA	81	N	6.517051
303	5KPF	MET	80	C	6.052117
304	5KPF	MET	80	N	6.347030
305	5KPF	CYS	17	CB	5.421849
306	5KPF	CYS	17	O	6.060536
307	5KPF	CYS	17	C	6.151005
308	5KPF	CYS	17	CA	6.490182
309	5KPF	HIS	18	ND1	4.055792
310	5KPF	PRO	30	CG	6.282517

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
311	5KPF	TYR	67	CZ	5.655118
312	5KPF	PRO	30	O	6.541035
313	5KPF	TYR	67	CE1	6.978646
314	5KPF	TYR	67	CD2	6.713518
315	5KPF	HIS	18	CG	4.117157
316	5KPF	PRO	30	N	6.286503
317	5KPF	GLY	29	C	6.305107
318	5KPF	GLY	29	CA	5.523623
319	5KPF	GLY	29	N	6.329067
320	5KPF	HIS	18	CB	5.533621
321	5KPF	CYS	14	SG	6.823397
322	5KPF	PRO	30	CD	5.626056
323	5KPF	HIS	18	N	6.382298
324	5KPF	CYS	14	O	6.293139
325	5KPF	CYS	14	C	6.993506
326	5KPF	CYS	14	CA	6.635959
327	5KPF	PHE	82	CD2	6.463558
328	5KPF	LEU	68	CD2	6.268124
329	5KPF	HIS	18	CA	6.470604
330	5KPF	MET	80	CA	5.255860
331	5KPF	CYS	17	SG	6.369154
332	5LFT	PHE	82	CG	6.356580
333	5LFT	HIS	18	CB	5.560732
334	5LFT	CYS	17	CB	5.313012
335	5LFT	PRO	71	CG	6.983064
336	5LFT	PHE	82	CD2	6.810043
337	5LFT	PHE	82	CD1	6.825499
338	5LFT	PHE	82	CB	5.873708
339	5LFT	MET	80	N	6.425431
340	5LFT	LEU	32	CD1	5.961830
341	5LFT	HIS	18	ND1	4.090804
342	5LFT	HIS	18	CG	4.147251
343	5LFT	HIS	18	CA	6.509885
344	5LFT	MET	80	CB	4.296074
345	5LFT	CYS	17	SG	6.343958

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
346	5LFT	TYR	67	OH	4.833680
347	5LFT	MET	80	CA	5.312127
348	5LFT	CYS	17	CA	6.413725
349	5LFT	TYR	67	CE2	5.462023
350	5LFT	PRO	30	CG	6.237908
351	5LFT	TYR	67	CE1	6.975655
352	5LFT	TYR	67	CD2	6.670309
353	5LFT	PRO	30	N	6.299143
354	5LFT	CYS	17	O	6.075895
355	5LFT	PRO	30	CD	5.671618
356	5LFT	HIS	18	CE1	2.966117
357	5LFT	HIS	18	CD2	3.029345
358	5LFT	LEU	32	CG	6.422071
359	5LFT	CYS	14	SG	6.824953
360	5LFT	CYS	14	O	6.214345
361	5LFT	CYS	14	C	6.937040
362	5LFT	CYS	14	CA	6.595268
363	5LFT	HIS	18	N	6.428173
364	5LFT	HIS	18	NE2	2.011687
365	5LFT	MET	80	CE	3.387584
366	5LFT	ALA	81	N	6.400723
367	5LFT	LEU	32	CD2	5.936545
368	5LFT	CYS	17	C	6.136386
369	5LFT	GLY	29	C	6.350219
370	5LFT	MET	80	SD	2.302768
371	5LFT	MET	80	C	6.108783
372	5LFT	LEU	68	CD2	6.315525
373	5LFT	GLY	29	CA	5.565072
374	5LFT	CYS	14	CB	6.420337
375	5LFT	GLY	29	N	6.229086
376	5LFT	MET	80	CG	3.456264
377	5LFT	TYR	67	CZ	5.655063
378	5LFT	PRO	30	O	6.508423
379	5LFT	MET	80	O	6.773883
380	5T8W	LEU	32	CG	6.343288

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
381	5T8W	PRO	30	CD	5.583175
382	5T8W	PRO	30	O	6.544388
383	5T8W	HIS	18	CE1	2.935155
384	5T8W	GLY	29	C	6.383245
385	5T8W	GLY	29	CA	5.637934
386	5T8W	HIS	18	CA	6.516657
387	5T8W	HIS	18	CB	5.562349
388	5T8W	HIS	18	ND1	4.065898
389	5T8W	HIS	18	CD2	3.019310
390	5T8W	HIS	18	CG	4.135070
391	5T8W	GLY	29	N	6.438759
392	5T8W	CYS	14	SG	6.847774
393	5T8W	CYS	14	CB	6.488403
394	5T8W	CYS	14	O	6.269192
395	5T8W	CYS	14	C	6.982236
396	5T8W	CYS	14	CA	6.649977
397	5T8W	MET	80	C	6.035762
398	5T8W	PHE	82	CD2	6.441516
399	5T8W	PHE	82	CD1	6.999821
400	5T8W	PHE	82	CG	6.253903
401	5T8W	PHE	82	CB	5.693194
402	5T8W	MET	80	CE	3.363519
403	5T8W	PHE	82	N	6.830508
404	5T8W	LEU	68	CD2	6.123569
405	5T8W	MET	80	N	6.419434
406	5T8W	ALA	81	N	6.484127
407	5T8W	HIS	18	N	6.453279
408	5T8W	MET	80	SD	2.281932
409	5T8W	MET	80	CG	3.400381
410	5T8W	MET	80	CB	4.224351
411	5T8W	MET	80	O	6.542416
412	5T8W	CYS	17	SG	6.407722
413	5T8W	TYR	67	OH	4.837618
414	5T8W	TYR	67	CZ	5.611609
415	5T8W	HIS	18	NE2	1.986642

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
416	5T8W	TYR	67	CE2	5.371411
417	5T8W	TYR	67	CE1	6.915964
418	5T8W	TYR	67	CD2	6.556593
419	5T8W	CYS	17	CB	5.457714
420	5T8W	PHE	82	CA	6.944552
421	5T8W	CYS	17	O	6.255528
422	5T8W	PRO	71	CG	6.909375
423	5T8W	MET	80	CA	5.276377
424	5T8W	PRO	30	CG	6.146734
425	5T8W	PRO	30	N	6.278789
426	5T8W	CYS	17	C	6.267167
427	5T8W	LEU	32	CD2	5.869608
428	5T8W	LEU	32	CD1	5.770229
429	5T8W	CYS	17	CA	6.555563
430	6VDQ	TYR	310	CD2	6.539713
431	6VDQ	PHE	320	CZ	5.684848
432	6VDQ	PHE	320	CE2	6.813343
433	6VDQ	PHE	320	CD1	6.496707
434	6VDQ	HIS	274	NE2	2.166653
435	6VDQ	HIS	274	ND1	4.253244
436	6VDQ	HIS	274	CB	5.649324
437	6VDQ	HIS	274	O	6.849876
438	6VDQ	HIS	274	CA	6.565180
439	6VDQ	CYS	317	SG	6.205606
440	6VDQ	CYS	317	CB	6.256735
441	6VDQ	HIS	274	CG	4.254245
442	6VDQ	PHE	320	CE1	5.492677
443	6VDQ	TRP	271	CH2	6.160079
444	6VDQ	TRP	271	CZ3	5.419019
445	6VDQ	TRP	271	CE3	6.062835
446	6VDQ	HIS	313	NE2	2.114046
447	6VDQ	HIS	313	CE1	3.148000
448	6VDQ	HIS	313	CD2	3.023814
449	6VDQ	HIS	313	CG	4.198200
450	6VDQ	HIS	313	CA	6.547666

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
451	6VDQ	HIS	313	ND1	4.222791
452	6VDQ	HIS	313	CB	5.589302
453	6VDQ	LEU	238	CD1	6.268885
454	6VDQ	LEU	238	CD2	6.550286
455	6VDQ	ILE	278	CD1	5.058554
456	6VDQ	HIS	274	CD2	3.095567
457	6VDQ	TYR	310	CE2	6.866809
458	6VDQ	LEU	277	CD2	6.506868
459	6VDQ	TYR	310	O	6.950794
460	6VDQ	TYR	310	CA	6.715562
461	6VDQ	THR	309	CG2	6.344180
462	6VDQ	HIS	274	CE1	3.169279
463	6VDQ	ILE	278	CG1	5.659029
464	6VDQ	THR	309	O	6.542999
468	6WZA	LEU	3	CG	6.517323
472	6WZA	PHE	65	CZ	6.255083
473	6WZA	MET	7	CG	3.480925
474	6WZA	HIS	102	CE1	3.359365
475	6WZA	LEU	3	O	6.635333
477	6WZA	HIS	102	NE2	2.320735
479	6WZA	HIS	102	CD2	3.189854
480	6WZA	LEU	10	CG	6.542974
481	6WZA	LEU	10	CB	6.311147
482	6WZA	HIS	102	CB	5.753321
483	6WZA	MET	7	O	5.917221
484	6WZA	HIS	102	ND1	4.435137
485	6WZA	HIS	102	CA	6.044747
486	6WZA	HIS	102	N	6.038413
487	6WZA	CYS	101	SG	6.288607
488	6WZA	CYS	101	CB	6.321072
489	6WZA	HIS	102	CG	4.383045
490	6WZA	MET	7	CB	4.280261
491	6WZA	CYS	101	C	6.757441
492	6WZA	LEU	10	CD1	5.349237
493	6WZA	MET	7	N	6.100669

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
494	6WZA	MET	7	CA	5.062932
495	6WZA	MET	7	CE	3.596894
496	6WZA	CYS	98	CA	5.725516
497	6WZA	MET	7	SD	2.492649
500	6WZA	CYS	98	SG	6.371545
501	6WZA	PHE	65	CE1	6.113498
502	6WZA	ARG	106	CG	6.665139
503	6WZA	ARG	106	CB	6.598225
505	6WZA	CYS	98	CB	5.537743
506	6WZA	LEU	3	CD2	6.809700
507	6WZA	LEU	3	CD1	6.828342
512	6WZA	MET	7	C	5.961312
513	6WZA	CYS	98	O	5.328723
515	6WZA	CYS	98	C	5.907987
520	6XNK	TYR	67	CD2	6.665357
521	6XNK	LYS	79	CE	3.037596
522	6XNK	TYR	67	HH	3.927833
523	6XNK	HIS	18	CB	5.436966
524	6XNK	TYR	67	HE2	4.676997
525	6XNK	TYR	67	HD2	6.800590
526	6XNK	LYS	79	HZ3	2.551045
527	6XNK	LYS	79	HZ2	1.278291
528	6XNK	LYS	79	HZ1	1.995026
529	6XNK	HIS	18	HE1	3.048190
530	6XNK	HIS	18	HD2	3.102772
531	6XNK	TYR	67	OH	4.722027
532	6XNK	LYS	79	HD2	3.476914
533	6XNK	LYS	79	HG3	4.729055
534	6XNK	LYS	79	HG2	5.367169
535	6XNK	HIS	18	H	6.514246
536	6XNK	LYS	79	HB2	5.945551
537	6XNK	HIS	18	CE1	2.845379
538	6XNK	HIS	18	CD2	2.886147
539	6XNK	LYS	79	NZ	1.966787
540	6XNK	HIS	18	CG	4.011526

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
541	6XNK	LYS	79	CD	3.847428
542	6XNK	LYS	79	CG	4.937653
543	6XNK	LYS	79	CB	6.116794
544	6XNK	HIS	18	CA	6.391595
545	6XNK	HIS	18	N	6.261778
546	6XNK	CYS	17	HB3	5.126034
547	6XNK	CYS	17	HB2	4.702452
548	6XNK	CYS	17	H	6.789989
549	6XNK	CYS	17	SG	6.384909
550	6XNK	CYS	17	CB	5.389003
551	6XNK	CYS	17	O	6.219656
552	6XNK	VAL	83	HG22	6.016615
553	6XNK	CYS	17	CA	6.469164
554	6XNK	GLY	29	C	6.293575
555	6XNK	VAL	83	CG2	6.186346
556	6XNK	TYR	67	CZ	5.655553
557	6XNK	CYS	14	HB3	5.236316
558	6XNK	CYS	14	HB2	6.786422
559	6XNK	CYS	14	HA	5.764442
560	6XNK	ILE	75	HG22	6.120135
561	6XNK	ILE	75	HG21	6.372387
562	6XNK	CYS	14	CB	6.135863
563	6XNK	CYS	14	O	6.219435
564	6XNK	CYS	14	C	6.877037
565	6XNK	CYS	14	CA	6.452203
566	6XNK	VAL	83	HG23	5.947690
567	6XNK	ILE	75	CG2	6.745580
568	6XNK	CYS	17	C	6.147917
569	6XNK	CYS	14	SG	6.735718
570	6XNK	VAL	83	HG21	5.865730
571	6XNK	LYS	79	HB3	6.554712
572	6XNK	GLY	29	H	6.329482
573	6XNK	PRO	30	HD3	6.090082
574	6XNK	PRO	30	HG3	6.407879
575	6XNK	PRO	30	HG2	5.676877

Table B.10: HEC: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
576	6XNK	PRO	30	CD	5.582001
577	6XNK	PRO	30	O	6.463050
578	6XNK	LEU	32	HG	6.383475
579	6XNK	PRO	30	N	6.232837
580	6XNK	GLY	29	HA3	4.597674
581	6XNK	GLY	29	CA	5.523654
582	6XNK	GLY	29	N	6.320921
583	6XNK	THR	28	HG22	6.983672
584	6XNK	HIS	18	ND1	3.958847
585	6XNK	PRO	30	HD2	4.620017
586	6XNK	LYS	79	HE3	2.992305
587	6XNK	LYS	79	HE2	3.779843
588	6XNK	PRO	30	CG	6.129220
589	6XNK	HIS	18	HD1	4.737228
590	6XNK	HIS	18	HB3	5.911807
591	6XNK	HIS	18	HB2	5.544422
592	6XNK	HIS	18	NE2	1.863057
593	6XNK	GLY	29	HA2	5.656172
594	6XNK	TYR	67	CE2	5.467347
595	6XNK	LEU	32	HD23	6.635463
596	6XNK	LEU	32	HD22	6.414908
597	6XNK	LEU	32	HD21	5.128961
598	6XNK	LEU	32	HD13	6.311844
599	6XNK	LEU	32	HD12	6.462496
600	6XNK	LEU	32	HD11	4.997047
601	6XNK	LYS	79	HD3	4.436220
602	6XNK	HIS	18	HA	6.481555
603	6XNK	LEU	32	CD2	6.069933
604	6XNK	LEU	32	CD1	5.956808
605	6XNK	LEU	32	CG	6.498159
606	6XNK	TYR	67	CE1	6.991656

Table B.11: SRM: All Distances, Atoms to Fe

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1	1ZJ8	ALA	468	N	6.774896
2	1ZJ8	CYS	467	C	5.622542
3	1ZJ8	SER	466	C	6.380682
4	1ZJ8	ARG	166	NH1	5.881161
5	1ZJ8	ASN	465	O	6.329793
6	1ZJ8	CYS	467	SG	2.739867
7	1ZJ8	ASN	465	C	6.729615
8	1ZJ8	ARG	97	NH2	4.715261
9	1ZJ8	CYS	467	CB	3.891589
10	1ZJ8	ARG	97	NH1	5.483193
11	1ZJ8	ARG	97	CZ	5.570784
12	1ZJ8	ARG	97	NE	6.762447
13	1ZJ8	CYS	467	O	5.620446
14	1ZJ8	ASN	465	CG	6.852489
18	1ZJ8	CYS	467	CA	4.572359
20	1ZJ8	CYS	467	N	5.409755
21	1ZJ8	GLN	134	OE1	6.870508
22	1ZJ8	LYS	209	NZ	4.794331
23	1ZJ8	LYS	209	CE	5.713878
24	1ZJ8	ASN	465	CB	6.117299
25	1ZJ8	TYR	69	OH	6.963349
26	1ZJ8	SER	466	O	6.698175
27	1ZJ8	LYS	207	NZ	4.097986
28	1ZJ8	LYS	207	CE	5.582174
29	1ZJ8	LYS	207	CD	6.158637
30	1ZJ8	ASN	465	ND2	6.919459
31	1ZJ8	ARG	166	CZ	6.942231
32	1ZJ8	ASP	129	OD1	6.873987
33	2AKJ	LYS	224	CE	5.100975
34	2AKJ	ARG	179	NH2	6.024724
35	2AKJ	ARG	179	CZ	6.635201
36	2AKJ	ARG	179	NE	6.152980
37	2AKJ	ARG	109	NH1	4.778753
38	2AKJ	ARG	109	CZ	5.550228
39	2AKJ	THR	142	OG1	6.814343

Table B.11: SRM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
40	2AKJ	GLY	487	N	6.536313
41	2AKJ	CYS	486	CB	3.620545
42	2AKJ	CYS	486	C	5.475420
43	2AKJ	CYS	486	CA	4.297414
44	2AKJ	CYS	486	N	5.041386
45	2AKJ	SER	485	O	6.571770
46	2AKJ	SER	485	C	6.120504
47	2AKJ	SER	485	N	6.820633
48	2AKJ	ASN	484	CG	6.359396
49	2AKJ	ASN	484	ND2	6.221626
50	2AKJ	ARG	109	NH2	5.430691
51	2AKJ	ASN	484	CB	5.666087
53	2AKJ	ARG	109	NE	6.736503
56	2AKJ	ASN	484	O	5.870993
57	2AKJ	ASN	484	C	6.293813
58	2AKJ	CYS	486	SG	2.307671
59	2AKJ	ASN	484	CA	6.671473
60	2AKJ	LYS	224	NZ	4.716982
61	2AKJ	CYS	486	O	5.661149
62	2AKJ	LYS	224	CD	6.060923
63	2AOP	ASN	116	OD1	6.627004
64	2AOP	LYS	217	NZ	4.913889
65	2AOP	LYS	217	CE	6.056179
66	2AOP	LYS	215	NZ	4.501462
72	2AOP	ARG	83	NE	6.690501
76	2AOP	LYS	215	CE	5.533781
77	2AOP	LYS	215	CD	6.529398
78	2AOP	GLY	484	N	6.751562
79	2AOP	CYS	483	SG	2.690933
80	2AOP	CYS	483	CB	3.618036
81	2AOP	CYS	483	O	5.925288
82	2AOP	CYS	483	C	5.701845
83	2AOP	CYS	483	CA	4.490487
84	2AOP	CYS	483	N	5.131759
85	2AOP	GLY	482	O	6.796617

Table B.11: SRM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
86	2AOP	GLY	482	C	6.207889
87	2AOP	GLY	482	N	6.927668
88	2AOP	ASN	481	ND2	6.951972
89	2AOP	ASN	481	CG	6.943965
90	2AOP	ASN	481	CB	6.133620
91	2AOP	ARG	83	NH2	4.987487
92	2AOP	ARG	83	NH1	6.116129
93	2AOP	ARG	83	CZ	5.827773
94	2AOP	ASN	481	O	6.234228
95	2AOP	ARG	153	NE	6.898322
96	2AOP	GLN	121	OE1	6.832109
97	2AOP	ASN	481	C	6.576284
101	3B0G	ALA	486	N	6.469408
102	3B0G	CYS	485	SG	2.376623
103	3B0G	CYS	485	CB	3.382867
104	3B0G	CYS	485	C	5.409016
105	3B0G	CYS	485	CA	4.239215
106	3B0G	CYS	485	N	5.000524
107	3B0G	THR	484	N	6.708903
108	3B0G	THR	484	O	6.455657
109	3B0G	THR	484	C	6.044003
110	3B0G	ASN	483	ND2	6.260093
111	3B0G	ASN	483	CB	5.581326
112	3B0G	ASN	483	O	5.719969
113	3B0G	ASN	483	C	6.160591
114	3B0G	ASN	483	CA	6.571598
115	3B0G	ASN	483	CG	6.338273
116	3B0G	THR	142	OG1	6.442796
117	3B0G	LYS	224	NZ	4.445729
118	3B0G	LYS	224	CE	5.810500
119	3B0G	LYS	224	CD	6.483612
120	3B0G	CYS	485	O	5.599037
121	3B0G	ARG	109	NH2	4.811922
122	3B0G	ARG	109	NH1	5.627262
123	3B0G	ARG	109	CZ	5.642075

Table B.11: SRM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
124	3B0G	ARG	109	NE	6.776761
125	3B0G	ARG	179	NH2	5.577161
126	3B0G	ARG	179	NH1	6.762778
127	3B0G	ARG	179	CZ	6.656967
133	3VKP	ASN	483	ND2	6.225943
134	3VKP	ASN	483	CA	6.569538
135	3VKP	ASN	483	CG	6.321808
136	3VKP	ALA	486	N	6.471195
137	3VKP	CYS	485	SG	2.364009
138	3VKP	CYS	485	CB	3.408761
139	3VKP	ASN	483	CB	5.554061
140	3VKP	CYS	485	O	5.618179
141	3VKP	CYS	485	C	5.409845
142	3VKP	CYS	485	CA	4.238243
143	3VKP	CYS	485	N	4.994489
144	3VKP	ASN	483	O	5.715338
145	3VKP	THR	484	C	6.044406
146	3VKP	THR	484	N	6.724690
147	3VKP	LYS	224	NZ	4.409855
148	3VKP	ASN	483	C	6.176402
149	3VKP	LYS	224	CD	6.342866
150	3VKP	LYS	224	CE	5.747677
151	3VKP	ARG	109	NH1	5.589424
152	3VKP	ARG	109	NE	6.832542
154	3VKP	ARG	109	NH2	4.835137
156	3VKP	THR	484	O	6.469202
157	3VKP	ARG	109	CZ	5.654695
158	3VKP	ARG	179	NH2	5.498837
159	3VKP	ARG	179	NH1	6.700761
160	3VKP	ARG	179	CZ	6.584269
161	3VKP	THR	142	OG1	6.428882
163	3VLX	ASN	483	CB	5.627120
164	3VLX	ASN	483	O	5.731451
165	3VLX	ASN	483	C	6.191851
166	3VLX	ASN	483	CA	6.613790

Table B.11: SRM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
168	3VLX	CYS	485	O	5.588423
169	3VLX	LYS	224	CE	5.854496
170	3VLX	CYS	485	C	5.403377
171	3VLX	LYS	224	NZ	4.491458
172	3VLX	CYS	485	CA	4.231946
173	3VLX	THR	142	OG1	6.455248
174	3VLX	CYS	485	N	4.995353
175	3VLX	THR	484	O	6.438040
176	3VLX	ARG	109	NH2	4.710989
177	3VLX	ARG	109	NH1	5.616270
178	3VLX	ARG	109	CZ	5.584909
179	3VLX	ARG	179	NH2	5.589544
180	3VLX	ARG	179	NH1	6.741095
181	3VLX	THR	484	N	6.735887
182	3VLX	ARG	179	CZ	6.667895
184	3VLX	LYS	224	CD	6.469108
187	3VLX	CYS	485	SG	2.376707
188	3VLX	CYS	485	CB	3.405528
189	3VLX	THR	484	C	6.031697
190	3VLX	ASN	483	ND2	6.328925
191	3VLX	ARG	109	NE	6.717005
192	3VLX	ASN	483	CG	6.404243
193	3VLX	ALA	486	N	6.481752
194	3VLY	LYS	224	CE.A	5.823785
195	3VLY	LYS	224	CD.B	6.546563
196	3VLY	LYS	224	CD.A	6.611656
197	3VLY	THR	484	O	6.426986
198	3VLY	ARG	179	NH1	6.736275
199	3VLY	ARG	179	CZ	6.688035
200	3VLY	THR	484	N	6.766892
201	3VLY	CYS	485	CB	3.391003
202	3VLY	CYS	485	C	5.430226
203	3VLY	ASN	483	ND2	6.390751
204	3VLY	THR	484	C	6.049208
205	3VLY	ASN	483	CG	6.488689

Table B.11: SRM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
206	3VLY	ASN	483	CB	5.691757
207	3VLY	ASN	483	O	5.740901
208	3VLY	LYS	226	CE	6.147136
209	3VLY	CYS	485	SG	2.389916
210	3VLY	ARG	109	NH2	4.750497
211	3VLY	ARG	109	NH1	5.601167
212	3VLY	ARG	109	CZ	5.592635
213	3VLY	ARG	109	NE	6.737305
214	3VLY	ASN	483	C	6.218756
215	3VLY	THR	142	OG1	6.452740
216	3VLY	ASN	483	CA	6.667256
217	3VLY	ARG	179	NH2	5.624064
219	3VLY	CYS	485	CA	4.259251
221	3VLY	LYS	226	NZ	4.824118
224	3VLY	CYS	485	N	5.011053
227	3VLY	LYS	224	CE.B	5.780367
228	3VLY	CYS	485	O	5.614114
230	3VLY	LYS	224	NZ.B	4.516341
231	3VLY	LYS	224	NZ.A	4.549145
232	3VLY	ALA	486	N	6.503895
233	3VLZ	ARG	109	NH2	4.807371
234	3VLZ	ARG	109	NH1	5.527607
235	3VLZ	ARG	109	CZ	5.593093
236	3VLZ	ARG	109	NE	6.737774
237	3VLZ	LYS	224	NZ	4.481281
238	3VLZ	LYS	224	CE	5.919855
239	3VLZ	LYS	224	CD	6.403020
240	3VLZ	THR	142	OG1	6.394057
244	3VLZ	LYS	226	NZ	5.015077
248	3VLZ	ALA	486	N	6.507235
249	3VLZ	CYS	485	SG	2.447780
250	3VLZ	CYS	485	CB	3.377554
251	3VLZ	LYS	226	CE	6.267389
252	3VLZ	CYS	485	O	5.620470
253	3VLZ	CYS	485	C	5.428716

Table B.11: SRM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
255	3VLZ	CYS	485	CA	4.263342
256	3VLZ	CYS	485	N	5.029616
257	3VLZ	ARG	179	CZ	6.755330
258	3VLZ	THR	484	O	6.426261
259	3VLZ	THR	484	C	6.045580
260	3VLZ	THR	484	N	6.840780
261	3VLZ	ASN	483	ND2	6.328586
262	3VLZ	ASN	483	CG	6.460443
263	3VLZ	ASN	483	CB	5.694910
264	3VLZ	ARG	179	NH2	5.698279
265	3VLZ	ASN	483	O	5.673531
266	3VLZ	ASN	483	C	6.216891
267	3VLZ	ASN	483	CA	6.659583
268	3VLZ	ARG	179	NH1	6.844514
269	5H8V	LYS	276	CD	6.408382
273	5H8V	THR	156	OG1	6.490994
274	5H8V	TYR	106	OH	6.992106
275	5H8V	CYS	494	CB	6.918908
276	5H8V	GLN	161	NE2	6.725078
277	5H8V	LYS	276	NZ	4.815119
278	5H8V	ARG	124	NH2	4.739208
280	5H8V	ARG	124	CZ	5.660284
281	5H8V	ARG	124	NE	6.748784
283	5H8V	LYS	276	CE	6.192486
284	5H8V	ALA	545	N	6.528336
285	5H8V	CYS	544	SG	2.393592
286	5H8V	CYS	544	CB	3.390855
287	5H8V	CYS	544	O	5.393867
288	5H8V	CYS	544	C	5.349018
289	5H8V	CYS	544	CA	4.227622
290	5H8V	CYS	544	N	5.011213
291	5H8V	GLY	543	O	6.455442
292	5H8V	GLY	543	C	5.986396
293	5H8V	GLY	543	CA	6.921074
294	5H8V	GLY	543	N	6.589065

Table B.11: SRM: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
295	5H8V	ASN	542	ND2	6.949259
296	5H8V	ARG	193	NE	6.748373
297	5H8V	ASN	542	CG	6.876195
298	5H8V	ASN	542	CB	5.939255
299	5H8V	ASN	542	O	6.143777
300	5H8V	ASN	542	C	6.353431
301	5H8V	ASN	542	CA	6.843112
302	5H8V	ARG	124	NH1	5.776669
306	5H8V	LYS	278	NZ	4.887668
307	5H8V	LYS	278	CE	6.104035

Table B.12: VERDOHEME: All Distances, Atoms to Fe

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
1	2ZVU	GLU	29	CA	6.550605
2	2ZVU	SER	142	CB	5.056016
3	2ZVU	SER	142	O	6.834314
4	2ZVU	SER	142	C	5.791933
5	2ZVU	SER	142	CA	6.079128
6	2ZVU	PHE	207	CE2	5.564495
7	2ZVU	SER	142	N	6.689489
8	2ZVU	ALA	28	CB	6.962159
9	2ZVU	ASP	140	N	6.674210
10	2ZVU	GLY	139	C	5.456061
11	2ZVU	GLY	139	CA	4.644464
12	2ZVU	GLU	29	CB	5.706315
13	2ZVU	GLY	139	N	5.698486
14	2ZVU	GLU	29	N	6.647271
15	2ZVU	HIS	25	C	6.543308
16	2ZVU	GLU	29	OE2	6.184195
17	2ZVU	THR	135	O	6.765195

Table B.12: VERDOHEME: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
18	2ZVU	GLU	29	OE1	6.021925
19	2ZVU	GLY	139	O	5.263773
20	2ZVU	GLU	29	CD	6.037613
21	2ZVU	HIS	25	NE2	2.139802
22	2ZVU	GLU	29	CG	6.403560
23	2ZVU	HIS	25	CE1	3.183117
24	2ZVU	HIS	25	CD2	3.046508
25	2ZVU	HIS	25	ND1	4.258746
26	2ZVU	HIS	25	CG	4.227114
27	2ZVU	GLY	143	O	6.662887
28	2ZVU	HIS	25	CB	5.615299
29	2ZVU	HIS	25	O	6.094479
30	2ZVU	LEU	138	O	6.138327
31	2ZVU	HIS	25	CA	6.320898
32	2ZVU	PHE	207	CD2	6.783590
33	2ZVU	GLY	144	N	5.902504
34	2ZVU	LEU	138	C	6.361209
35	2ZVU	GLY	143	C	5.752517
36	2ZVU	GLY	143	CA	4.732326
37	2ZVU	GLY	143	N	4.596848
38	2ZVU	SER	142	OG	5.838988
39	2ZVU	PHE	207	CZ	5.764150
40	3MOO	HIS	20	ND1	4.253818
41	3MOO	HIS	20	CG	4.226474
42	3MOO	HIS	20	CB	5.622946
43	3MOO	HIS	20	O	6.158634
44	3MOO	HIS	20	C	6.569026
45	3MOO	HIS	20	CD2	3.045131
46	3MOO	HIS	20	CA	6.339432
47	3MOO	HIS	20	CE1	3.180759
48	3MOO	GLY	140	N	6.027517
49	3MOO	PHE	201	CZ	6.094516
50	3MOO	GLY	139	O	6.646135
51	3MOO	GLY	139	C	5.759376
52	3MOO	GLY	139	CA	4.646653

Table B.12: VERDOHEME: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
53	3MOO	GLY	139	N	4.423907
54	3MOO	SER	138	OG	5.753269
55	3MOO	SER	138	CB	4.836803
56	3MOO	SER	138	O	6.682551
57	3MOO	SER	138	C	5.593718
58	3MOO	VAL	131	O	6.796515
59	3MOO	SER	138	N	6.590947
61	3MOO	GLU	24	OE2	5.384554
63	3MOO	GLU	24	CD	6.389236
64	3MOO	GLU	24	CG	6.455965
65	3MOO	GLU	24	CB	6.226563
66	3MOO	ASP	136	N	6.778611
67	3MOO	GLY	135	O	5.140137
68	3MOO	GLY	135	C	5.487685
69	3MOO	GLY	135	CA	4.772529
70	3MOO	GLY	135	N	5.753634
72	3MOO	PHE	201	CE1	5.823481
73	3MOO	LEU	134	O	5.948257
74	3MOO	LEU	134	C	6.251889
75	3MOO	SER	138	CA	5.863632
76	3MOO	HIS	20	NE2	2.136783
77	3MOO	GLU	24	CA	6.921235
110	1TWN	SER	142	OG	6.202751
210	1TWN	SER	142	CB	5.278474
310	1TWN	SER	142	O	6.521440
410	1TWN	SER	142	C	5.608074
510	1TWN	SER	142	CA	6.079325
610	1TWN	SER	142	N	6.525137
71	1TWN	GLY	139	O	4.637782
81	1TWN	GLY	139	CA	4.688754
91	1TWN	GLY	139	N	5.966079
101	1TWN	ASP	140	N	6.273979
111	1TWN	LEU	138	C	6.568643
121	1TWN	GLU	29	OE2	5.896688
131	1TWN	GLY	139	C	5.078584

Table B.12: VERDOHEME: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
141	1TWN	GLU	29	CD	6.031038
151	1TWN	GLU	29	CG	5.943908
161	1TWN	GLU	29	OE1	6.622662
171	1TWN	THR	135	O	6.865192
181	1TWN	PHE	207	CZ	6.131186
191	1TWN	HIS	25	NE2	2.125073
201	1TWN	HIS	25	CE1	3.033509
211	1TWN	HIS	25	CD2	3.170330
221	1TWN	HIS	25	ND1	4.177685
231	1TWN	HIS	25	CG	4.274450
241	1TWN	HIS	25	CB	5.705445
251	1TWN	HIS	25	O	6.316837
261	1TWN	HIS	25	C	6.784392
271	1TWN	HIS	25	CA	6.472605
281	1TWN	PHE	207	CE2	5.765491
291	1TWN	PHE	207	CD2	6.894472
301	1TWN	LEU	138	O	6.230476
311	1TWN	GLY	144	N	6.024952
321	1TWN	GLY	143	O	6.416018
331	1TWN	GLY	143	C	5.619207
341	1TWN	GLY	143	CA	4.451235
351	1TWN	GLY	143	N	4.438393
361	1TWR	HIS	25	ND1	4.147733
371	1TWR	SER	142	CA	6.432405
381	1TWR	ASP	140	N	6.553790
391	1TWR	GLY	139	O	4.904275
401	1TWR	GLY	139	C	5.360673
411	1TWR	GLY	139	CA	4.975291
421	1TWR	GLY	139	N	6.237301
431	1TWR	LEU	138	O	6.380104
441	1TWR	LEU	138	C	6.779436
451	1TWR	HIS	25	CB	5.956100
461	1TWR	GLU	29	OE2	5.747718
471	1TWR	GLU	29	OE1	6.976207
481	1TWR	GLU	29	CD	6.414442

Table B.12: VERDOHEME: All Distances, Atoms to Fe *(continued)*

	PDB_ID	Residue_Code	Residue_Number	Atom	Distance
491	1TWR	GLU	29	CG	6.930261
501	1TWR	PHE	207	CZ	6.416044
511	1TWR	PHE	207	CE2	5.938056
521	1TWR	PHE	207	CD2	6.989446
551	1TWR	HIS	25	NE2	2.360871
561	1TWR	HIS	25	CD2	3.578572
571	1TWR	HIS	25	CG	4.495311
581	1TWR	HIS	25	O	6.244702
591	1TWR	HIS	25	C	6.776047
60	1TWR	HIS	25	CA	6.610832
611	1TWR	GLY	143	C	6.723686
62	1TWR	GLY	143	CA	5.540835
631	1TWR	GLY	143	N	5.245156
641	1TWR	SER	142	CB	5.353755
651	1TWR	SER	142	C	6.273485
661	1TWR	SER	142	N	6.885149
671	1TWR	SER	142	OG	6.030291
681	1TWR	HIS	25	CE1	2.909126

B.3.2 Mean Distances of Each Residue in Binding Pocket

Table B.13: HEM: Mean Distances of Each Residue in Pocket

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
1N45	28	ALA	6.981230
2CJ0	31	ALA	5.440871
2CPO	31	ALA	5.505123
2J18	31	ALA	5.457126
1SY2	42	ALA	6.006055
3MVF	42	ALA	5.827660
3TGC	42	ALA	6.033598

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
2O6P	49	ALA	6.356063
4B8N	54	ALA	6.390793
1B5M	67	ALA	5.797296
1ICC	67	ALA	6.085233
1U9U	67	ALA	6.016697
2CJ0	71	ALA	6.531120
2CPO	71	ALA	6.539227
2J18	71	ALA	6.477348
3HX9	71	ALA	6.230664
4NL5	71	ALA	6.805378
4Y1Q	75	ALA	6.722226
1P3T	121	ALA	6.382367
3SIK	138	ALA	6.231014
3QZN	166	ALA	6.907969
2R7A	169	ALA	5.223004
6A2J	180	ALA	6.687029
2BHJ	191	ALA	6.261711
6A2J	220	ALA	5.986896
6A2J	259	ALA	6.937825
4MYP	282	ALA	6.581195
4MYP	293	ALA	6.207799
2Q6N	298	ALA	5.672036
4I3Q	305	ALA	5.305272
5VEU	305	ALA	6.219660
1ZVI	412	ALA	6.481380
2Q6N	442	ALA	6.935846
5VEU	447	ALA	6.667315
4I3Q	448	ALA	6.441232
4JET	40	ARG	5.660400
4XZD	40	ARG	5.892195
4Y1Q	40	ARG	5.725205
3SIK	54	ARG	6.090293
2FC2	61	ARG	6.072553
2FC2	65	ARG	6.459491
4CDP	100	ARG	5.360373

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
2J0P	102	ARG	5.002395
4UZV	105	ARG	6.689489
4MF9	112	ARG	5.056393
5GJ3	142	ARG	9.016294
4JET	144	ARG	6.239587
4XZD	144	ARG	6.335714
4Y1Q	144	ARG	6.425880
2BHJ	193	ARG	5.745098
2BHJ	197	ARG	6.221230
4I3Q	212	ARG	6.392849
1QHU	214	ARG	6.588734
1QJS	214	ARG	6.249190
6A2J	217	ARG	6.781589
5GJ3	241	ARG	5.542517
2IIZ	242	ARG	5.236889
1SI8	333	ARG	5.247624
2IPS	348	ARG	6.336679
7C74	348	ARG	6.274279
7DMR	348	ARG	6.250958
1IPH	411	ARG	5.321024
1ZVI	414	ARG	5.799426
1ZVI	418	ARG	6.259544
3HX9	7	ASN	9.030558
4NL5	7	ASN	5.402231
1B2V	41	ASN	6.894251
1DK0	41	ASN	6.870425
1P3T	118	ASN	6.625279
1SI8	127	ASN	6.666708
1IPH	201	ASN	6.396844
2BHJ	364	ASN	6.955669
2IPS	437	ASN	6.276979
7C74	437	ASN	6.653391
7DMR	437	ASN	6.591349
5VEU	440	ASN	6.408862
4I3Q	441	ASN	6.139159

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
1P3T	27	ASP	6.267807
2E2Y	64	ASP	6.865050
2IPS	108	ASP	5.870986
7C74	108	ASP	6.017401
7DMR	108	ASP	6.266021
5KZL	129	ASP	6.318347
1N45	140	ASP	6.389011
1VGI	140	ASP	6.566393
2IIZ	151	ASP	5.861207
4CDP	191	ASP	6.789427
2J0P	194	ASP	6.862392
1QHU	203	ASP	6.920576
1QJS	203	ASP	6.878437
2IIZ	284	ASP	6.598336
2CJ0	29	CYS	4.390905
2CPO	29	CYS	4.443549
2J18	29	CYS	4.359887
2FC2	62	CYS	4.482879
1P3T	113	CYS	6.881310
2BHJ	194	CYS	4.487497
1ZVI	415	CYS	4.181834
2Q6N	436	CYS	4.305637
5VEU	441	CYS	4.349464
4I3Q	442	CYS	4.085782
2IPS	105	GLN	5.981590
7C74	105	GLN	5.667218
7DMR	105	GLN	5.517249
5GJ3	141	GLN	9.940999
2R7A	253	GLN	6.081153
6A2J	258	GLN	5.803666
4MYP	292	GLN	6.537566
5KZL	19	GLU	5.803913
1N45	29	GLU	6.277510
1VGI	29	GLU	6.279863
5O1L	148	GLU	6.440638

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
2CJ0	183	GLU	5.716050
2CPO	183	GLU	5.799506
2J18	183	GLU	5.722472
1QHU	225	GLU	6.177350
1QJS	226	GLU	6.465511
2IPS	258	GLU	6.388898
7C74	258	GLU	6.258582
7DMR	258	GLU	6.172262
2Q6N	439	GLU	6.270464
1ZVI	592	GLU	6.601349
1B5M	41	GLY	5.388127
1ICC	41	GLY	5.723853
1U9U	41	GLY	5.723510
1B5M	42	GLY	6.533917
1ICC	42	GLY	6.657462
1U9U	42	GLY	6.689632
4B8N	50	GLY	5.464969
4B8N	51	GLY	6.462950
1B5M	62	GLY	6.365897
2FC2	64	GLY	5.882725
1P3T	116	GLY	5.737222
1P3T	120	GLY	4.843774
5KZL	128	GLY	5.130966
5KZL	132	GLY	5.705062
1N45	139	GLY	5.251379
1VGI	139	GLY	5.155470
1N45	143	GLY	5.882948
1VGI	143	GLY	5.279720
1VGI	144	GLY	5.974807
2R7A	170	GLY	5.922307
6A2J	179	GLY	5.548597
2BHJ	196	GLY	5.667103
2FC2	233	GLY	6.517575
6A2J	262	GLY	5.820895
4MYP	291	GLY	6.624699

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
2Q6N	299	GLY	6.518431
4I3Q	306	GLY	6.573103
2IPS	350	GLY	6.712596
7C74	350	GLY	6.606591
7DMR	350	GLY	6.694618
2BHJ	365	GLY	6.617587
1ZVI	417	GLY	5.404983
2Q6N	438	GLY	5.615678
5VEU	443	GLY	5.482822
4I3Q	444	GLY	5.222394
1ZVI	586	GLY	6.997972
5KZL	15	HIS	4.819650
1P3T	23	HIS	4.573926
1N45	25	HIS	4.545004
1VGI	25	HIS	4.646180
1B2V	32	HIS	4.667618
1DK0	32	HIS	4.556145
1DKH	32	HIS	5.099382
1B5M	39	HIS	4.456809
1ICC	39	HIS	4.542187
1U9U	39	HIS	4.589294
4B8N	48	HIS	4.479396
1SI8	54	HIS	5.688888
1SY2	59	HIS	4.045387
3MVF	59	HIS	4.066882
3TGC	59	HIS	4.100823
1B5M	63	HIS	4.211990
1ICC	63	HIS	4.451283
1U9U	63	HIS	4.417873
2SPL	64	HIS	5.889080
5CN5	64	HIS	5.804727
4B8N	71	HIS	4.416116
3VP5	72	HIS	4.371971
3HX9	75	HIS	4.195649
4NL5	75	HIS	4.473936

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
4JET	81	HIS	5.381133
4XZD	81	HIS	5.263108
4Y1Q	81	HIS	5.294289
1B2V	83	HIS	5.366599
1DK0	83	HIS	5.314133
1DKH	83	HIS	5.223800
2CN4	83	HIS	5.251875
3QZN	83	HIS	4.660500
2E2Y	93	HIS	4.514535
2SPL	93	HIS	4.578545
5CN5	93	HIS	4.575365
2E2Y	97	HIS	5.917056
2SPL	97	HIS	5.997752
5CN5	97	HIS	5.966408
4UZV	106	HIS	4.502311
2IPS	109	HIS	5.924623
7C74	109	HIS	5.952700
7DMR	109	HIS	5.699226
2VEB	120	HIS	4.471709
3QZZ	120	HIS	4.599066
3ZJS	120	HIS	4.427156
1IPH	128	HIS	5.713777
2O6P	134	HIS	6.496593
3VP5	149	HIS	4.350835
3QZN	168	HIS	6.973181
4CDP	193	HIS	4.417630
2J0P	196	HIS	4.310325
5O1L	198	HIS	4.305405
5O1M	198	HIS	4.392715
4MF9	209	HIS	4.606487
1QHU	213	HIS	4.734866
1QJS	213	HIS	4.696712
6A2J	216	HIS	4.601722
1QHU	222	HIS	6.740296
2IIZ	224	HIS	4.533607

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
1QHU	265	HIS	4.200094
1QJS	266	HIS	4.484379
6A2J	278	HIS	4.655598
2IPS	351	HIS	4.125792
7C74	351	HIS	4.494179
7DMR	351	HIS	4.201640
3HX9	9	ILE	9.558396
4NL5	9	ILE	5.756873
4JET	30	ILE	6.988601
2O6P	48	ILE	5.365972
4B8N	55	ILE	5.758462
2FC2	63	ILE	6.106378
2E2Y	68	ILE	5.517060
3VP5	71	ILE	6.407016
2E2Y	99	ILE	6.130795
2SPL	99	ILE	6.223033
5CN5	99	ILE	6.410362
2E2Y	107	ILE	6.704700
2SPL	107	ILE	6.505472
5CN5	107	ILE	6.767432
4UZV	111	ILE	5.897899
2Q6N	114	ILE	6.560571
2VEB	116	ILE	6.573571
3QZZ	116	ILE	6.472356
3ZJS	116	ILE	6.518950
2O6P	121	ILE	6.852081
3SIK	129	ILE	6.189129
3SIK	131	ILE	6.481115
2VEB	137	ILE	6.361213
3QZZ	137	ILE	6.393964
3ZJS	137	ILE	6.315026
3QZN	159	ILE	5.866079
3QZN	164	ILE	6.384201
2BHJ	195	ILE	6.216303
2FC2	214	ILE	6.545905

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
5O1L	222	ILE	6.024951
5O1M	222	ILE	6.241067
2IIZ	225	ILE	6.430481
5O1L	227	ILE	6.973430
4CDP	252	ILE	6.178209
2J0P	255	ILE	6.197370
6A2J	265	ILE	6.271826
4MF9	268	ILE	6.092502
2Q6N	363	ILE	6.794813
2Q6N	435	ILE	6.531691
5VEU	442	ILE	6.119535
4I3Q	443	ILE	5.985023
2CJ0	32	LEU	5.757197
2CPO	32	LEU	5.913058
2J18	32	LEU	5.760472
1B5M	46	LEU	5.848737
1ICC	46	LEU	5.941384
1U9U	46	LEU	5.958763
1SY2	57	LEU	6.145372
3MVF	57	LEU	6.242544
3TGC	57	LEU	6.147624
4B8N	70	LEU	6.456250
1B2V	77	LEU	6.429830
1DK0	77	LEU	6.502332
1DKH	77	LEU	6.345588
2CN4	77	LEU	6.548785
4UZV	79	LEU	6.352126
2E2Y	89	LEU	6.167984
2SPL	89	LEU	6.446644
5CN5	89	LEU	6.607510
4CDP	90	LEU	6.499175
4UZV	102	LEU	6.801707
2E2Y	104	LEU	6.384225
2SPL	104	LEU	6.518599
5CN5	104	LEU	6.517400

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
1P3T	119	LEU	6.709401
1SY2	123	LEU	5.902915
3MVF	123	LEU	5.891492
3TGC	123	LEU	5.908675
5KZL	127	LEU	6.731689
1SY2	133	LEU	6.241713
3MVF	133	LEU	6.341681
3TGC	133	LEU	6.315080
5KZL	136	LEU	6.422701
1N45	138	LEU	6.717099
1VGI	138	LEU	6.110494
2VEB	142	LEU	6.331426
3QZZ	142	LEU	6.534813
3ZJS	142	LEU	6.289922
1N45	147	LEU	6.115862
2R7A	167	LEU	6.508147
5O1L	171	LEU	5.743071
2IIZ	255	LEU	6.075868
2R7A	257	LEU	5.559331
2IIZ	286	LEU	5.566800
2IPS	417	LEU	6.792313
2IPS	433	LEU	5.458537
7C74	433	LEU	5.275537
7DMR	433	LEU	5.225161
2Q6N	437	LEU	5.864970
3VP5	145	LYS	5.832567
5O1M	167	LYS	5.125712
3QZN	84	MET	6.337233
1B2V	140	MET	6.218846
1DK0	140	MET	6.185917
1DKH	140	MET	6.519598
2CN4	140	MET	5.816277
4JET	147	MET	5.810508
4XZD	147	MET	6.297861
4Y1Q	147	MET	6.115760

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
4UZV	151	MET	5.908059
4CDP	241	MET	6.340896
2J0P	244	MET	6.821994
4MF9	257	MET	6.826627
5VEU	444	MET	6.285199
4I3Q	445	MET	5.975507
3HX9	23	PHE	8.679990
4NL5	23	PHE	5.580423
2SPL	29	PHE	6.129536
1B5M	35	PHE	5.848448
1ICC	35	PHE	6.276818
1U9U	35	PHE	6.094672
2SPL	43	PHE	5.815167
5CN5	43	PHE	5.981197
4B8N	44	PHE	6.120000
4JET	50	PHE	6.875792
4Y1Q	50	PHE	6.555816
4UZV	53	PHE	6.941930
2CJ0	57	PHE	6.484645
2CPO	57	PHE	6.473913
2J18	57	PHE	6.534471
1B5M	58	PHE	6.096500
1ICC	58	PHE	6.182239
4B8N	67	PHE	6.248829
4UZV	67	PHE	5.984317
1SY2	68	PHE	6.098374
3MVF	68	PHE	6.146303
3TGC	68	PHE	6.152796
2VEB	74	PHE	6.405384
3QZZ	74	PHE	6.218919
3ZJS	74	PHE	6.270262
3VP5	76	PHE	6.844578
4JET	77	PHE	6.310922
4XZD	77	PHE	6.275751
4Y1Q	77	PHE	6.412846

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
2VEB	93	PHE	5.810118
3QZZ	93	PHE	6.033470
3ZJS	93	PHE	5.922481
2CJ0	103	PHE	6.182880
2CPO	103	PHE	6.396792
2J18	103	PHE	6.235843
3VP5	112	PHE	6.509162
4UZV	119	PHE	5.820671
1SI8	132	PHE	6.553242
1SI8	140	PHE	5.575451
2VEB	145	PHE	6.211153
3QZZ	145	PHE	6.192963
3ZJS	145	PHE	6.059949
1P3T	181	PHE	5.974488
2CJ0	186	PHE	5.833496
2CPO	186	PHE	5.891089
2J18	186	PHE	5.882819
5KZL	195	PHE	6.351090
2J0P	199	PHE	6.468406
1IPH	206	PHE	6.665963
1N45	207	PHE	5.975984
1VGI	207	PHE	6.238995
1IPH	214	PHE	5.767678
2FC2	231	PHE	6.129726
4CDP	243	PHE	5.994465
2J0P	246	PHE	6.155004
2IIZ	257	PHE	5.749045
4MF9	259	PHE	5.680334
7C74	347	PHE	6.478230
7DMR	347	PHE	6.671472
2BHJ	363	PHE	5.980185
2Q6N	429	PHE	6.192258
5VEU	434	PHE	6.084164
4I3Q	435	PHE	6.161681
1ZVI	584	PHE	6.009975

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
2CJ0	28	PRO	6.127671
2CPO	28	PRO	6.018197
2J18	28	PRO	6.103023
2CJ0	30	PRO	5.960531
2CPO	30	PRO	6.017188
2J18	30	PRO	5.936382
1B5M	40	PRO	6.032548
1ICC	40	PRO	6.016737
1U9U	40	PRO	6.149502
4B8N	49	PRO	6.182011
1SI8	315	PRO	6.539721
1IPH	393	PRO	6.703993
2Q6N	428	PRO	6.945175
5VEU	433	PRO	6.574196
4I3Q	434	PRO	6.893037
1B2V	42	SER	6.443386
1DK0	42	SER	6.540219
1DKH	42	SER	6.070312
2FC2	59	SER	6.581787
2E2Y	92	SER	6.454585
2SPL	92	SER	6.650791
5CN5	92	SER	6.529632
1P3T	117	SER	5.531584
5GJ3	124	SER	10.238794
5KZL	131	SER	6.438631
1N45	142	SER	6.525024
1VGI	142	SER	5.700272
4MYP	205	SER	6.655356
6A2J	261	SER	6.949581
1QHU	266	SER	6.680148
1QJS	267	SER	6.730283
1IPH	414	SER	6.728176
1DK0	33	THR	6.991008
2R7A	52	THR	5.945515
2E2Y	67	THR	6.891096

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
3VP5	68	THR	6.164947
4XZD	82	THR	6.830323
1B2V	84	THR	6.798527
1DK0	84	THR	6.799510
1DKH	84	THR	6.267175
2CN4	84	THR	6.804573
1SY2	121	THR	6.333312
3MVF	121	THR	6.595150
3TGC	121	THR	6.343084
3VP5	130	THR	5.980868
1N45	135	THR	6.713859
1VGI	135	THR	6.883314
5O1M	168	THR	6.373467
6A2J	178	THR	6.772182
5O1L	194	THR	6.305648
5O1M	194	THR	6.409916
4MF9	208	THR	6.202558
5O1L	230	THR	6.574103
5O1M	230	THR	6.603918
2Q6N	302	THR	5.748396
4I3Q	309	THR	6.214341
5VEU	309	THR	5.895842
2E2Y	43	TRP	5.845537
2FC2	56	TRP	5.737975
3QZZ	60	TRP	6.491833
3ZJS	60	TRP	6.366999
3HX9	66	TRP	7.852796
4NL5	66	TRP	6.235302
2R7A	68	TRP	6.192116
1QHU	171	TRP	6.147194
1QJS	171	TRP	6.211700
2VEB	185	TRP	5.717992
3QZZ	185	TRP	6.111800
3ZJS	185	TRP	5.960798
2BHJ	188	TRP	6.049049

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
2CJ0	213	TRP	6.764355
2J18	213	TRP	6.782850
2FC2	234	TRP	6.837576
1QHU	267	TRP	5.987630
1QJS	268	TRP	6.230710
2BHJ	366	TRP	6.764735
1ZVI	409	TRP	5.660275
1ZVI	587	TRP	6.843603
1SY2	40	TYR	5.887937
3MVF	40	TYR	6.759408
3TGC	40	TYR	5.967215
2O6P	52	TYR	6.682161
2CN4	55	TYR	6.806239
4JET	55	TYR	6.877273
4XZD	55	TYR	6.821652
4Y1Q	55	TYR	6.699820
1SY2	58	TYR	6.964531
1U9U	58	TYR	6.232812
3ZJS	61	TYR	6.548411
2R7A	67	TYR	4.159993
1B2V	75	TYR	4.251885
1DK0	75	TYR	4.346840
1DKH	75	TYR	4.792830
2CN4	75	TYR	4.345054
4JET	75	TYR	4.420106
4XZD	75	TYR	4.329954
3QZN	87	TYR	6.251729
3VP5	91	TYR	6.574739
2O6P	132	TYR	4.055037
2O6P	136	TYR	5.148558
3SIK	136	TYR	4.260470
1B2V	137	TYR	6.232518
1DK0	137	TYR	6.186950
1DKH	137	TYR	6.409147
2CN4	137	TYR	6.142879

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
3SIK	140	TYR	5.120136
5GJ3	140	TYR	7.520130
3QZN	170	TYR	5.718488
1QHU	204	TYR	6.239544
1QJS	204	TYR	6.225721
5GJ3	239	TYR	4.170326
4MYP	280	TYR	4.465249
4MYP	289	TYR	5.900895
1SI8	337	TYR	3.976560
1IPH	415	TYR	4.218561
1P3T	26	VAL	6.716946
1SY2	36	VAL	6.479806
3TGC	36	VAL	6.135653
1B2V	37	VAL	5.425221
1DK0	37	VAL	5.400636
1DKH	37	VAL	5.642973
1B5M	45	VAL	5.846522
1ICC	45	VAL	5.992035
1U9U	45	VAL	6.500194
1SI8	53	VAL	6.238869
3HX9	53	VAL	10.092943
4NL5	53	VAL	5.909472
1B5M	61	VAL	6.074911
1ICC	61	VAL	5.726742
1U9U	61	VAL	6.163696
2SPL	68	VAL	5.598014
5CN5	68	VAL	5.556498
4B8N	75	VAL	6.033658
2VEB	89	VAL	5.917494
3QZZ	89	VAL	5.927268
3ZJS	89	VAL	5.790982
2O6P	119	VAL	6.176593
5KZL	124	VAL	6.607237
1SI8	125	VAL	6.016899
1IPH	127	VAL	6.256166

Table B.13: HEM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
3VP5	131	VAL	5.568423
3VP5	148	VAL	6.888565
5O1L	152	VAL	6.293389
5O1M	152	VAL	6.250877
3QZN	161	VAL	6.290827
6A2J	175	VAL	6.202413
6A2J	182	VAL	6.679490
4CDP	192	VAL	5.600764
2J0P	195	VAL	6.307524
5O1L	197	VAL	6.648164
5O1M	197	VAL	6.631076
1IPH	199	VAL	6.294207
2IIZ	228	VAL	5.315815
2BHJ	346	VAL	6.643571
2IPS	354	VAL	6.655642
5VEU	369	VAL	6.886497
1ZVI	416	VAL	5.960795

Table B.14: HEC: Mean Distances of Each Residue in Pocket

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
5KPF	81	ALA	6.517051
5LFT	81	ALA	6.400723
5T8W	81	ALA	6.484127
3EAH	147	ALA	6.240842
2BC5	106	ARG	5.961420
6WZA	106	ARG	6.631682
1BBH	129	ARG	5.790808
3EAH	149	ARG	5.803314
3EAH	153	ARG	6.514542
2BC5	99	ASN	6.936196

Table B.14: HEC: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
3X15	12	CYS	6.451594
5KPF	14	CYS	6.631432
5LFT	14	CYS	6.598389
5T8W	14	CYS	6.647516
6XNK	14	CYS	6.275930
2BH5	15	CYS	6.513509
3X15	15	CYS	6.178945
5KPF	17	CYS	6.098545
5LFT	17	CYS	6.056595
5T8W	17	CYS	6.188739
6XNK	17	CYS	5.903640
1W2L	18	CYS	6.554906
2BH5	18	CYS	6.369197
1W2L	21	CYS	6.223591
2BC5	98	CYS	5.957326
6WZA	98	CYS	5.774303
2BC5	101	CYS	6.394766
6WZA	101	CYS	6.455707
1BBH	121	CYS	5.737156
1BBH	124	CYS	6.272059
3EAH	150	CYS	4.247423
6VDQ	317	CYS	6.231170
1S56	58	GLN	6.005777
1BBH	17	GLU	6.940695
3X15	24	GLY	6.352237
5KPF	29	GLY	6.052599
5LFT	29	GLY	6.048126
5T8W	29	GLY	6.153313
6XNK	29	GLY	5.786913
1W2L	31	GLY	6.565877
2BH5	36	GLY	6.126048
3EAH	152	GLY	5.627214
3X15	16	HIS	4.360557
5KPF	18	HIS	4.310334
5LFT	18	HIS	4.342999

Table B.14: HEC: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
5T8W	18	HIS	4.334295
6XNK	18	HIS	4.599701
2BH5	19	HIS	4.283790
1W2L	22	HIS	4.350769
1S56	81	HIS	4.475028
2BC5	102	HIS	4.186908
6WZA	102	HIS	4.440577
1BBH	125	HIS	4.218890
6VDQ	274	HIS	4.500421
6VDQ	313	HIS	4.120545
3X15	30	ILE	6.412845
1W2L	61	ILE	6.839545
6XNK	75	ILE	6.412701
1S56	86	ILE	5.878780
6VDQ	278	ILE	5.358791
2BC5	3	LEU	6.742954
6WZA	3	LEU	6.697674
2BC5	10	LEU	6.154091
6WZA	10	LEU	6.067786
5KPF	32	LEU	6.145036
5LFT	32	LEU	6.106815
5T8W	32	LEU	5.994375
6XNK	32	LEU	6.085909
2BH5	39	LEU	5.728784
1S56	54	LEU	5.947501
5KPF	68	LEU	6.268124
5LFT	68	LEU	6.315525
5T8W	68	LEU	6.123569
6VDQ	238	LEU	6.409586
6VDQ	277	LEU	6.506868
6XNK	79	LYS	3.938274
2BH5	100	LYS	4.313747
2BC5	7	MET	4.661903
6WZA	7	MET	4.611608
1BBH	19	MET	6.049470

Table B.14: HEC: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
1W2L	76	MET	4.403618
1S56	77	MET	6.187616
5KPF	80	MET	4.692154
5LFT	80	MET	4.757864
5T8W	80	MET	4.693021
1W2L	34	PHE	5.935685
3X15	44	PHE	6.024333
1S56	46	PHE	5.938368
2BC5	65	PHE	6.201901
6WZA	65	PHE	6.184290
5KPF	82	PHE	6.311357
5LFT	82	PHE	6.466458
5T8W	82	PHE	6.527249
2BH5	102	PHE	6.736126
3EAH	319	PHE	6.137327
6VDQ	320	PHE	6.121894
3X15	25	PRO	6.252857
5KPF	30	PRO	6.184028
5LFT	30	PRO	6.179273
5T8W	30	PRO	6.138272
6XNK	30	PRO	5.900245
1W2L	32	PRO	6.457693
2BH5	37	PRO	6.202537
5KPF	71	PRO	6.976183
5LFT	71	PRO	6.983064
5T8W	71	PRO	6.909375
1W2L	77	PRO	6.071845
2BH5	83	PRO	6.953188
1W2L	60	SER	6.470812
6XNK	28	THR	6.983672
6VDQ	309	THR	6.443589
3EAH	144	TRP	5.647844
6VDQ	271	TRP	5.880644
3EAH	322	TRP	6.529256
1BBH	16	TYR	4.795494

Table B.14: HEC: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
1S56	33	TYR	6.252015
1BBH	58	TYR	6.554347
5KPF	67	TYR	5.922923
5LFT	67	TYR	5.919346
5T8W	67	TYR	5.858639
6XNK	67	TYR	5.613420
2BH5	79	TYR	5.535216
1W2L	80	TYR	6.249808
6VDQ	310	TYR	6.768220
1W2L	75	VAL	6.753821
1S56	80	VAL	6.205932
2BH5	80	VAL	6.887770
6XNK	83	VAL	6.004096
1S56	94	VAL	6.626107
1S56	126	VAL	6.029592
3EAH	151	VAL	6.103944

Table B.15: SRM: Mean Distances of Each Residue in Pocket

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
1ZJ8	468	ALA	6.774896
3B0G	486	ALA	6.469408
3VKP	486	ALA	6.471195
3VLX	486	ALA	6.481752
3VLY	486	ALA	6.503895
3VLZ	486	ALA	6.507235
5H8V	545	ALA	6.528336
2AOP	83	ARG	5.905472
1ZJ8	97	ARG	5.632921
2AKJ	109	ARG	5.624044
3B0G	109	ARG	5.714505

Table B.15: SRM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
3VKP	109	ARG	5.727950
3VLX	109	ARG	5.657293
3VLY	109	ARG	5.670401
3VLZ	109	ARG	5.666461
5H8V	124	ARG	5.731236
2AOP	153	ARG	6.898322
1ZJ8	166	ARG	6.411696
2AKJ	179	ARG	6.270969
3B0G	179	ARG	6.332302
3VKP	179	ARG	6.261289
3VLX	179	ARG	6.332845
3VLY	179	ARG	6.349458
3VLZ	179	ARG	6.432708
5H8V	193	ARG	6.748373
2AOP	116	ASN	6.627004
1ZJ8	465	ASN	6.589731
2AOP	481	ASN	6.568014
3B0G	483	ASN	6.105308
3VKP	483	ASN	6.093849
3VLX	483	ASN	6.149563
3VLY	483	ASN	6.199685
3VLZ	483	ASN	6.172324
2AKJ	484	ASN	6.180565
5H8V	542	ASN	6.517505
1ZJ8	129	ASP	6.873987
1ZJ8	467	CYS	4.642760
2AOP	483	CYS	4.593058
3B0G	485	CYS	4.334547
3VKP	485	CYS	4.338921
3VLX	485	CYS	4.333556
3VLY	485	CYS	4.349260
3VLZ	485	CYS	4.361247
2AKJ	486	CYS	4.400598
5H8V	494	CYS	6.918908
5H8V	544	CYS	4.294361

Table B.15: SRM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
2AOP	121	GLN	6.832109
1ZJ8	134	GLN	6.870508
5H8V	161	GLN	6.725078
2AOP	482	GLY	6.644058
2AOP	484	GLY	6.751562
2AKJ	487	GLY	6.536313
5H8V	543	GLY	6.487994
1ZJ8	207	LYS	5.279599
1ZJ8	209	LYS	5.254105
2AOP	215	LYS	5.521547
2AOP	217	LYS	5.485034
2AKJ	224	LYS	5.292960
3B0G	224	LYS	5.579947
3VKP	224	LYS	5.500133
3VLX	224	LYS	5.605021
3VLY	224	LYS	5.637976
3VLZ	224	LYS	5.601385
3VLY	226	LYS	5.485627
3VLZ	226	LYS	5.641233
5H8V	276	LYS	5.805329
5H8V	278	LYS	5.495851
1ZJ8	466	SER	6.539429
2AKJ	485	SER	6.504302
2AKJ	142	THR	6.814343
3B0G	142	THR	6.442796
3VKP	142	THR	6.428882
3VLX	142	THR	6.455248
3VLY	142	THR	6.452740
3VLZ	142	THR	6.394057
5H8V	156	THR	6.490994
3B0G	484	THR	6.402854
3VKP	484	THR	6.412766
3VLX	484	THR	6.401875
3VLY	484	THR	6.414362
3VLZ	484	THR	6.437540

Table B.15: SRM: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
1ZJ8	69	TYR	6.963349
5H8V	106	TYR	6.992106

Table B.16: VERDOHEME: Mean Distances of Each Residue in Pocket

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
2ZVU	28	ALA	6.962159
3MOO	136	ASP	6.778611
2ZVU	140	ASP	6.674210
3MOO	24	GLU	6.275511
2ZVU	29	GLU	6.221641
3MOO	135	GLY	5.288496
2ZVU	139	GLY	5.265696
3MOO	139	GLY	5.369017
3MOO	140	GLY	6.027517
2ZVU	143	GLY	5.436145
2ZVU	144	GLY	5.902504
3MOO	20	HIS	4.614778
2ZVU	25	HIS	4.603252
3MOO	134	LEU	6.100073
2ZVU	138	LEU	6.249768
3MOO	201	PHE	5.958999
2ZVU	207	PHE	6.037412
3MOO	138	SER	5.886820
2ZVU	142	SER	6.048311
2ZVU	135	THR	6.765195
3MOO	131	VAL	6.796515
1TWN	140	ASP	6.273979
1TWR	140	ASP	6.553790
1TWN	29	GLU	6.123574
1TWR	29	GLU	6.517157

Table B.16: VERDOHEME: Mean Distances of Each Residue in Pocket *(continued)*

PDB_ID	Residue_Number	Residue_Code	Mean_Distance
1TWN	139	GLY	5.092800
1TWR	139	GLY	5.369385
1TWN	143	GLY	5.231213
1TWR	143	GLY	5.836559
1TWN	144	GLY	6.024952
1TWN	25	HIS	4.673370
1TWR	25	HIS	4.786588
1TWN	138	LEU	6.399559
1TWR	138	LEU	6.579770
1TWN	207	PHE	6.263716
1TWR	207	PHE	6.447849
1TWN	142	SER	6.035867
1TWR	142	SER	6.195017
1TWN	135	THR	6.865192

B.4 Volume and Surface Areas

B.4.1 Tables of Volume and Surface Areas, Distance Cutoff 7A

Table B.17: HEM: Volume and Surface Areas, Cutoff 7A

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

Table B.17: HEM: Volume and Surface Areas, Cutoff 7A *(continued)*

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

Table B.17: HEM: Volume and Surface Areas, Cutoff 7A *(continued)*

PDB_ID	Volume_Data	HEM_Excluded_SA	HEM_Accessible_SA	Pocket_Excluded_SA	Pocket_Accessible_SA
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.18: HEC: Volume and Surface Areas, Cutoff 7A

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

Table B.18: HEC: Volume and Surface Areas, Cutoff 7A *(continued)*

PDB_ID	Volume_Data	HEC_Excluded_SA	HEC_Accessible_SA	Pocket_Excluded_SA	Pocket_Accessible_SA
3X15	823.59	496.328	802.584	5722.90	7493.62
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.19: SRM: Volume and Surface Areas, Cutoff 7A

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.20: VERDOHEME: Volume and Surface Areas, Cutoff 7A

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.4.2 Tables of Volume and Surface Areas, Distance Cutoff 5A

Table B.21: HEM: Volume and Surface Areas, Cutoff 5A

PDB_ID	Volume_Data	HEM_Excluded_SA	HEM_Accessible_SA	Pocket_Excluded_SA	Pocket_Accessible_SA
1B2V	825.86	502.042	820.988	7276.09	8232.60
1B5M	644.19	490.050	800.780	4695.01	5512.20
1DK0	873.82	505.258	837.157	7237.94	8217.58
1DKH	910.74	509.042	828.131	7402.34	8175.94
1ICC	904.56	499.585	811.357	5079.72	6028.23
1IPH	976.97	501.603	814.652	33983.80	34094.40
1N45	836.59	560.384	983.238	9944.50	10779.30
1P3T	930.51	509.939	829.611	9530.67	10410.80
1QHU	1214.00	573.686	1002.160	18503.10	18257.20
1QJS	1093.20	573.266	1000.380	18588.40	18584.10
1SI8	762.27	646.643	1184.070	23711.20	25120.40
1SY2	898.89	501.850	817.749	8960.76	9610.23
1U9U	677.19	496.132	813.773	4675.76	5632.32
1VGI	820.91	577.234	1002.530	9615.29	10248.20

Table B.21: HEM: Volume and Surface Areas, Cutoff 5A *(continued)*

PDB_ID	Volume_Data	HEM_Excluded_SA	HEM_Accessible_SA	Pocket_Excluded_SA	Pocket_Accessible_SA
1ZVI	994.62	701.091	1129.540	19918.60	20968.20
2BHJ	1183.70	836.576	1290.530	20102.30	20762.60
2CJ0	798.44	2653.180	4835.280	12749.60	12892.20
2CN4	439.81	576.760	961.348	9617.23	11917.70
2CPO	884.75	1846.490	3329.540	13081.60	12995.60
2E2Y	902.38	811.270	1607.370	7531.94	8240.75
2FC2	1048.40	1011.190	1669.900	18383.50	18552.10
2IIZ	925.88	731.342	1393.160	13651.70	14031.40
2IPS	935.82	618.252	1075.560	27760.50	25814.10
2J0P	925.87	1030.510	1873.810	15192.90	15871.10
2J18	788.31	1962.990	3556.340	12675.10	12779.00
2O6P	675.40	499.017	822.121	6234.84	7200.43
2Q6N	971.08	644.365	1040.080	20051.10	19747.50
2R7A	889.50	507.098	845.182	11255.10	12389.00
2SPL	882.22	589.706	1029.660	7588.36	8105.94
2VEB	845.18	762.309	1454.750	9840.72	10401.80
3HX9	1792.70	785.442	1168.200	5819.08	7189.03
3MVF	1087.90	576.502	1009.950	8559.24	9573.08
3QZN	724.66	664.858	1221.330	6133.24	7179.49
3QZZ	903.93	496.950	825.255	8523.59	9708.28
3SIK	478.73	498.621	823.565	6495.38	7739.06
3TGC	926.51	524.380	853.710	8712.77	9181.94
3VP5	875.01	602.790	1050.820	9801.82	10810.80
3ZJS	842.79	528.419	860.137	9568.10	10130.40
4B8N	812.96	569.302	990.216	4560.39	5458.66
4CAT	583.88	484.341	778.502	28372.40	36788.30
4CDP	996.51	1425.050	3141.090	14733.50	15887.40
4I3Q	1044.70	510.623	845.108	21946.50	21093.70
4JET	908.16	495.992	818.131	7887.81	8695.85
4MF9	1041.70	488.695	790.732	15669.80	16791.30
4MYP	559.54	963.019	1834.680	6285.40	7351.53
4NL5	1052.20	576.669	1003.400	5715.52	6894.72
4UZV	1115.10	526.584	844.058	7378.28	8322.74
4XZD	853.44	498.788	816.032	8028.32	8752.50

Table B.21: HEM: Volume and Surface Areas, Cutoff 5A *(continued)*

PDB_ID	Volume_Data	HEM_Excluded_SA	HEM_Accessible_SA	Pocket_Excluded_SA	Pocket_Accessible_SA
4Y1Q	835.77	494.939	806.960	7905.84	8785.04
5CN5	901.87	663.162	1223.640	7629.45	8117.34
5GJ3	1095.50	756.603	1131.670	11394.00	12591.80
5KZL	870.61	483.760	805.567	9662.03	10431.00
5O1L	1111.80	801.519	1447.270	15538.20	16876.00
5O1M	1053.40	493.850	799.331	16096.90	15912.50
5VEU	838.05	993.578	1502.660	20900.80	20425.90
6A2J	857.55	6183.450	9902.920	14870.30	15888.00
7C74	904.00	497.527	820.381	26111.40	25094.20
7DMR	853.80	1049.750	1916.950	26004.00	24563.80

Table B.22: HEC: Volume and Surface Areas, Cutoff 5A

PDB_ID	Volume_Data	HEC_Excluded_SA	HEC_Accessible_SA	Pocket_Excluded_SA	Pocket_Accessible_SA
1BBH	894.91	514.130	829.817	6441.44	7514.06
1S56	1012.10	643.733	1075.840	6711.26	7477.96
1W2L	715.73	702.711	1240.680	5042.58	5485.50
2BC5	933.67	569.905	997.324	5489.91	6306.02
2BH5	757.38	508.637	844.494	6359.51	6975.70
3EAH	1022.70	993.430	1697.130	18413.40	19313.80
3X15	600.12	496.328	802.584	5722.90	7493.62
5KPF	747.68	568.036	1007.680	5485.51	6155.84
5LFT	803.97	1720.870	2719.000	5539.47	6315.96
5T8W	806.94	511.519	848.952	5755.48	6458.40
6VDQ	789.70	510.534	846.299	13399.60	14076.40
6WZA	879.49	713.997	1095.240	5529.40	6385.75
6XNK	1579.90	499.687	835.610	6737.92	8143.17

Table B.23: SRM: Volume and Surface Areas, Cutoff 5A

PDB_ID	Volume_Data	SRM_Excluded_SA	SRM_Accessible_SA	Pocket_Excluded_SA	Pocket_Accessible_SA
1ZJ8	1605.5	656.508	1036.43	20388.7	21432.8
2AKJ	1539.8	659.667	1041.00	21673.6	20933.7
2AOP	1057.2	682.170	1045.18	18119.8	18016.0
3B0G	1104.0	666.995	1054.40	21496.8	21033.9
3VKP	1096.4	675.050	1049.85	21279.3	20964.9
3VLX	1098.5	667.013	1052.76	21470.0	21037.0
3VLY	1040.1	675.293	1046.41	21476.6	21022.1
3VLZ	1162.3	676.360	1051.40	21433.5	20901.8
5H8V	1153.7	685.850	1052.56	22885.9	22713.3

Table B.24: VERDOHEME: Volume and Surface Areas, Cutoff 5A

PDB_ID	Volume_Data	VERDOHEME_EXCLUDED_SA	VERDOHEME_ACCESSIBLE_SA	POCKET_EXCLUDED_SA	POCKET_ACCESSIBLE_SA
2ZVU	875.9	560.791	969.143	9633.81	10317.3
3MOO	705.2	870.228	1772.07	9371.88	10170.3
1TWN	1103.5	448.81	759.632	9966.97	10896.8
1TWR	1002.9	469.982	783.313	9854.01	10775.6

B.5 All Planar Angles

Table B.25: 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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.25: HEM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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.26: 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

Table B.26: HEC: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
3EAH	147	ALA	6.240842	65.476	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
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
6VDQ	317	CYS	6.231170	64.036	CYS
1S56	58	GLN	6.005777	46.505	GLN
1BBH	17	GLU	6.940695	44.648	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

Table B.26: HEC: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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
6VDQ	274	HIS	4.500421	76.928	HIS
6VDQ	313	HIS	4.120545	68.371	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
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

Table B.26: HEC: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
6VDQ	238	LEU	6.409586	33.875	LEU
6VDQ	277	LEU	6.506868	55.119	LEU
6XNK	79	LYS	3.938274	74.591	LYS
2BH5	100	LYS	4.313747	77.818	LYS
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
3EAH	319	PHE	6.137327	43.608	PHE
6VDQ	320	PHE	6.121894	69.729	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
1W2L	60	SER	6.470812	29.839	SER

Table B.26: HEC: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
6XNK	28	THR	6.983672	89.881	THR
6VDQ	309	THR	6.443589	76.554	THR
3EAH	144	TRP	5.647844	55.208	TRP
6VDQ	271	TRP	5.880644	62.992	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

Table B.27: 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

Table B.27: SRM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.27: SRM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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
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

Table B.27: SRM: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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.28: 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
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

Table B.28: VERDOHEME: All Planar Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Angle	Residue_Code.y
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.6 All CA-CB-Fe Angles

Table B.29: 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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.29: HEM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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.30: 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

Table B.30: HEC: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.30: HEC: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.30: HEC: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.30: HEC: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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.31: 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
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

Table B.31: SRM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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
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

Table B.31: SRM: All CA-CB-Fe Angles *(continued)*

PDB_ID	Residue_Number	Residue_Code.x	Mean_Distance	Residue_Code.y	Angle
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.32: 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

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