

**COMPUTER SIMULATION OF DYNAMIC BEHAVIORS OF
MICROTUBULE PROTOFILAMENTS**

An Undergraduate Research Scholars Thesis

by

JAMES EDWARD GONZALES II

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Dr. Wonmuk Hwang

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ABSTRACT

Computer Simulation of Dynamic Behaviors of Microtubule Protofilaments

James Edward Gonzales II
Department of Biomedical Engineering
Texas A&M University

Research Advisor: Dr. Wonmuk Hwang
Department of Biomedical Engineering
Texas A&M University

The purpose of this study was to explore and understand the behavior of microtubule protofilaments (MT PFs) in a dynamic environment through molecular dynamics simulations. MTs play a vital role in various cellular processes such as: transport of materials within cells, cell structure and stability, and cell division. During normal cellular processes, MTs continuously polymerize and depolymerize depending on the nucleotide present in the end tubulin, either guanosine triphosphate (GTP) or guanosine diphosphate (GDP). While previous research has found that the nucleotide at the end of the filament is responsible, it is unclear why.

To understand the effects of the nucleotide state, molecular dynamics simulations were performed on two different conformations of a MT PF system. One conformation contained tubulin bound only to GTP and the other conformation contained tubulin bound to both GTP and GDP. Both conformations were simulated in two different sizes, as a 2-dimer and 4-dimer MT PF, which resulted in 4 unique systems. The 2-dimer systems were simulated for 400 nanoseconds (ns), and the 4-dimer systems were simulated for 210 ns.

The difference in simulation times is due to computation time limitations. The trajectories of these simulations were analyzed using a method developed in our lab, to quantify the mechanical properties of MT PFs as an elastic rod in order to easily predict the mechanical behavior of the MT PF. Additionally, an analysis of the non-polar and polar contacts found between tubulin was performed to see the chemical effect of the nucleotide state on the mechanical properties of MT PFs.

It was found that the mechanical properties of a MT PF can be accurately quantified as an elastic rod. The results from our analysis showed differences in these mechanical properties between the two conformations. We believe that the specific contacts present in the tubulin interfaces are likely responsible for the changes observed in mechanical properties between the conformations. It was also found that although the bending stiffness analysis shows promising results, longer simulations need to be obtained to make definitive claims based on these properties.

DEDICATION

To Cheryl & Jim Gonzales, my mother and father as well as the rest of my family. Without their continuous love and support none of this would be possible, and to my amazing friends that provided constant support and motivation.

ACKNOWLEDGMENTS

I would like to thank Dr. Wonmuk Hwang, without the mentorship, guidance, and opportunities he provided I would not have been able to complete this project. I would also like to thank Ana Chang-Gonzalez and Jie Shi for helping me with my many questions throughout this project. Finally, I would like to thank Texas A&M University's High Performance Research Computing Facilities, without the use of their supercomputers this project would not have been possible.

NOMENCLATURE

MT(s)	Microtubule(s)
PF(s)	Protofilament(s)
GTP	Guanosine Triphosphate
GDP	Guanosine Diphosphate
MD	Molecular Dynamics
ns	Nanoseconds
K	Kelvin
CHARMM	Chemistry at HARvard Macromolecular Mechanics
VMD	Visual Molecular Dynamics
Resid(s)	Residue ID(s)
Segname(s)	Segment Name(s)
psf	Protein Structure File
cor	Atom Coordinate File
pdb	Protein Databank File
PBC	Periodic Boundary Condition
CM	Center of Mass
RCSB PDB	Research Collaboratory for Structural Bioinformatics Protein Data Bank

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1. INTRODUCTION AND LITERATURE REVIEW

1.1 Introduction

Over the past few decades, there has been a growing interest in studying MTs as they have been shown to be a target for various disease treatments such as cancer and Alzheimer's Disease [1] [2]. However, not much is known about what drives the dynamic behaviors of MTs. The purpose of this project was to discover and outline some of the mechanical and chemical differences between the two different conformations of MT PFs.

1.1.1 Introduction to Microtubules

MTs play a vital role in various cellular processes, such as: transport of materials within cells, cell structure and stability, and namely, cell division [3]. MTs are comprised of α & β -tubulin. These tubulin bind together to form what is known as tubulin dimers. These tubulin dimers bind in such a way that the α -tubulin of one dimer binds to the β -tubulin of another dimer. This process continues and forms the PFs seen in MTs [4]. MTs are comprised of 13 PFs around, and have two distinct “ends”, known as the plus (+) end and the minus (-) end. The names of the ends do not denote charge, however, serve as a naming convention. MTs are generally stable at the (-) end, which acts as an anchor point allowing for elongation. In contrast, the (+) end of a MT is extremely unstable and dynamic. The general structure of a MT can be seen in Figure 1.1.

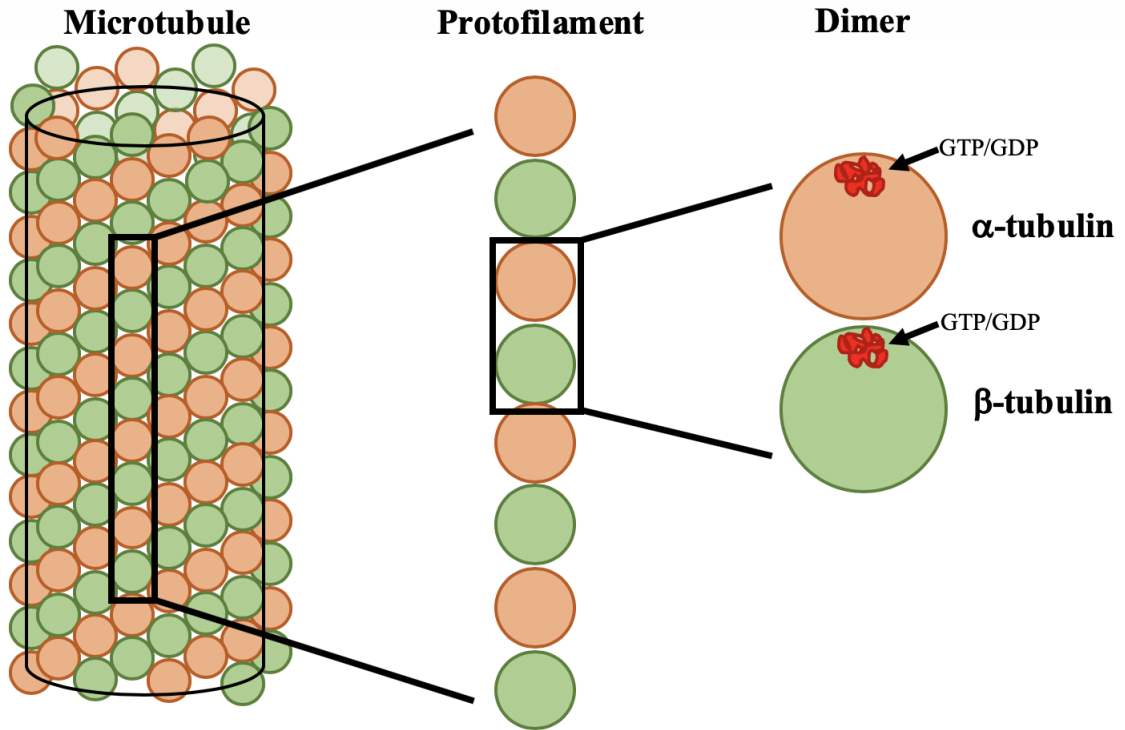


Figure 1.1: Breakdown of the structures which comprise a microtubule

1.1.2 *Dynamic Behaviors of Microtubules*

MTs are constantly elongating (polymerizing) and shortening (depolymerizing) through a process known as dynamic instability [5]. In dynamic instability, polymerization is known as “rescue” and depolymerization is known as “catastrophe”. During rescue, tubulin dimers and oligomers (small chains of tubulin dimers) bind to the (+) end of the MT. This binding takes place between the initial α -tubulin of the tubulin dimer or oligomer and an exposed β -tubulin of a MT [6]. During catastrophe, the MT loses stability and rapidly depolymerizes from the (+) end. Not much is known about this phenomenon, however, it is known that the main controller is the nucleotide present in the (+) end tubulin [7]. Both α - & β -tubulin are bound to either guanosine-triphosphate (GTP) or guanosine-diphosphate

(GDP). It has been shown through previous experiments that when the β -tubulin at the plus (+) end of a MT contains GTP the MT is able to polymerize, however, when GTP is hydrolyzed into GDP the MT begins rapid depolymerization [6].

1.2 Project Summary

Through our project, we wished to explore and better understand the dynamic behaviors of MT PFs. We approach this by outlining the various differences between the two conformations described above in a dynamic environment by utilizing molecular dynamics (MD) simulations. Previous atomistic MD simulations have been performed on MTs [8] [9], however these simulations failed to find a difference in properties depending on nucleotide state, so the problem is still unsolved. Our project introduces a better understanding of the differences in dynamic properties of MT PFs as well as some potential reasons for their conformational changes.

In our project, we performed MD simulations of two conformations of MT PFs. One conformation of the MT PF contained both α - & β -tubulin bound only to GTP, and another PF with α -tubulin bound to GTP, and β -tubulin bound to GDP [4]. Both of these conformations were simulated as systems containing 2 tubulin dimers (2-dimer systems), as well as systems containing 4 tubulin dimers (4-dimer systems). Both of the 2-dimer systems were simulated for 400 ns, and both 4-dimer systems were simulated for 210 ns.

From the simulations in this study, we were able to quantify the mechanical properties of MT PFs as elastic rods more accurately than had been previously done, establish contacts present between tubulin in a dynamic environment, and show potential evidence of how small chemical differences between the two conformations of MT PFs affected larger mechanical properties. In the following sections of this thesis we discuss, in detail, the procedure and results of the simulations, future directions and applications of this project, and some concluding remarks.

2. MATERIALS AND METHODS

2.1 Constructing a Usable Model for Microtubule Protofilaments

In generating an atomistic model for our protein, we utilized the expansive library of proteins found in the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB). The reported structures which we used were 3RYF (α - & β -tubulin bound to GTP) and 3RYI (α -tubulin bound to GTP & β -tubulin bound to GDP) [4]. The structures used from RCSB have 2.52 Å and 2.4 Å resolutions, respectively, which are high enough resolutions for the generation of atomistic models of MT PFs. In order to achieve such a high resolution structure, the MT PFs needed to be stabilized. This was achieved by binding the MT PFs to a RB3 Stathmin-like domain complex [4]. However, this introduced molecules which are not native to MTs *in vivo*. In order to acquire a usable model of a MT PF *in vivo*, we removed the stabilizing molecules and generated a structure with a file format which could be easily used by CHARMM. This process is outlined in detail in the following sections. The simulation methods for the 2-dimer and 4-dimer systems are the exact same except for building the structure which is discussed below.

2.1.1 2-Dimer System

When building the 2-dimer system, both 3RYF and 3RYI had the same extraneous molecules and followed the same procedure except 3RYI contained GDP as well as GTP. Initially, we separated the entire protein databank file into separate components (main protein, nucleotides, and surface water) in their own individual files. From this point, we began to assign specific labeling and naming conventions to allow for ease of analyzing specific pieces of the entire protein structure. This included defining residue IDs (resids), which are numbers associated with groups of atoms which comprise the amino acids in the

protein, and segment names (segnames), which are labels for groups of molecules which make up different domains of the MT PF. To clarify, a segname categorizes molecules present in various domains of the protein, where resids mark a specific amino acid residue which may have the same segname as other amino acid residues. This process was done for all three of the main components: the main protein, the nucleotides, and the surface water in the structure. Next, we used a CHARMM script which defined the specific segnames, and number of molecules in the specific segment (e.g. the surface waters of the first tubulin are segment TIP3A of which there are 118). After defining these parameters, the script then reads the coordinates, which were separated from the original RCSB PDB file, to generate the corresponding protein structure file (psf) and protein databank file (pdb). The psf characterizes the bonds and structure of the specific molecule, and the pdb file contains the 3-dimensional spatial coordinates of the atoms in the molecule. This was repeated for all of the surface waters and nucleotides in the PF.

Once the nucleotides and surface waters were built, the main protein was constructed. This was done by utilizing a C++ code written by Dr. Wonmuk Hwang, which took the atoms from the RCSB PDB file and rewrote them into the same pdb format as the water and nucleotides pdb files. After this script was ran, the amino acid sequence was checked to ensure it was translated correctly. From this point, the amino acid sequence of the first and second tubulin were copied into another CHARMM script which then read the sequence, renamed the segments to match a previous convention used, where the initial α -tubulin was labeled TA00 and the corresponding β -tubulin was labeled TB00. The following tubulin were labeled with increasing numerical numbers (i.e. TA01, TB01, etc.). After defining the names for the tubulin, the coordinates were read from the files generated from the C++ code, and then built using CHARMM algorithms.

These CHARMM algorithms formed the native bonds in the protein, and attempted to fill in missing coordinates which may not have been reported due to imaging limitations.

Unfortunately, this process does not always maintain the integrity of the coordinates for the extremely mobile outer loops of the protein. CHARMM may have inadvertently altered the coordinates of these atoms slightly. To resolve this issue, we used a program in Python called Modeller which randomly selects coordinates of atoms in specific amino acid residues from a range identified by the user to alter, then returns the different configurations found. This is done in an attempt to achieve the lowest energy state of the filled in coordinates for these residues. We selected the range of amino acid residues which CHARMM filled coordinates in to modify. With potentially altered coordinates, natural bonds may not have been formed. To ensure the most accurate model possible, the protein was then “held” using a harmonic constraint, except for the modified atoms, and then energy minimized to ensure natural bonds were formed. A psf and pdb file were generated for the minimized structure of the main protein, nucleotides, and surface waters. Finally, we used a CHARMM script which read in each psf and pdb and then wrote a complete psf and coordinate (cor) file containing the complete structure of the protein. This final structure contained only native atoms of a MT PF *in vivo*, and was the model which was used throughout the rest of the project. In Figure 2.1 below, α -tubulin are highlighted in orange and β -tubulin are highlighted in green of the 2-dimer system of 3RYF.

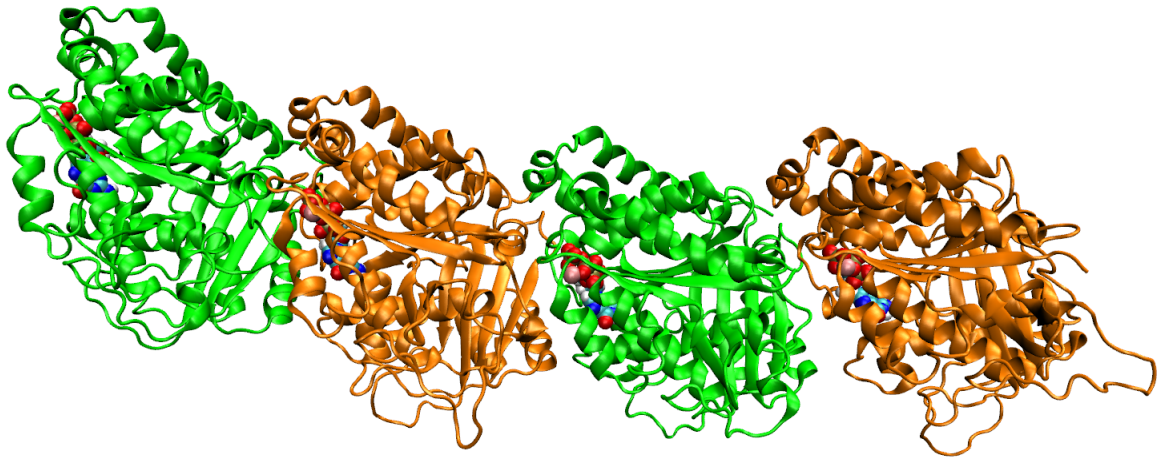


Figure 2.1: 2-dimer microtubule protofilament system (Tubulin from right to left: TA00, TB00, TA01, TB01)

2.1.2 4-Dimer System

To enhance our project and gather more data and results, we decided to carefully create a model of a 4-dimer MT PF from the 2-dimer model described in the previous section. Various stages of the structure we generated can be seen in Figure 2.2. Due to the delicate nature of proteins, one cannot simply create an exact copy of the protein and append it to the original structure. To accurately extend the filament to twice the size of the imaged structure, we selected specific tubulin to duplicate, align, and natively append to the original structure. We began by duplicating the entire filament, removing the final β -tubulin of the original structure, renaming the segments following the convention described earlier, and then appended the structures into the same file. After combining the structures, we then used a CHARMM script which used the root mean square position of the α -carbons of two tubulin dimers to align, ensuring the most accurate alignment possible. Once aligned, the two tubulin which contained native intra-dimer (between an α - & β -tubulin) or inter-dimer (between a β -tubulin and the next α -tubulin) interfaces were conserved while the

other two tubulin were removed.

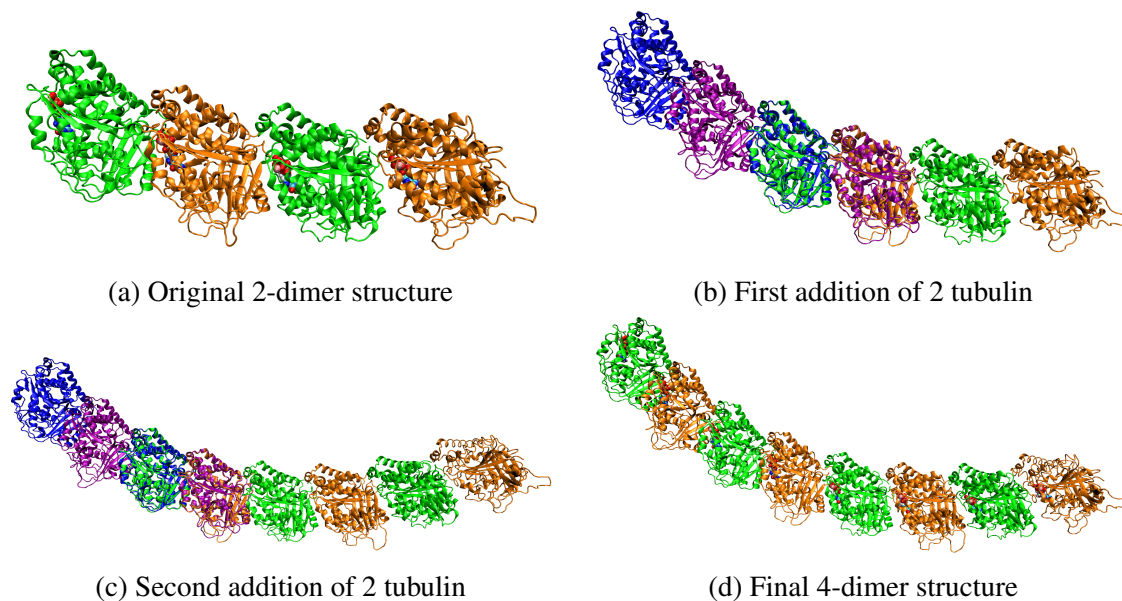


Figure 2.2: Figures (b) & (c) show the original structure with α -tubulin highlighted in orange, and β -tubulin highlighted in green, and the appended structure with α -tubulin highlighted in purple, and β -tubulin highlighted in blue

After these tubulin were added, the artificial interfaces were annealed, by again “holding” the other tubulin with a harmonic constraint, and allowing the new tubulin to form natural contacts. This process was then repeated to add the final two tubulin. This resulted in a structure containing 7 tubulin (4 α - & 3 β -tubulin). The final β -tubulin from the original 2-dimer structure (TB01) was then renamed to TB03 and added to the end of the structure. The final β -tubulin was then annealed as the other tubulin were previously to result in the final 4-dimer structure used in our simulations. Figure 2.2 shows structures of intermediate structures throughout building the 4-dimer system, and Figure 2.3 shows the completed 4-dimer system of 3RYF, with α -tubulin highlighted in orange and β -tubulin highlighted in green.

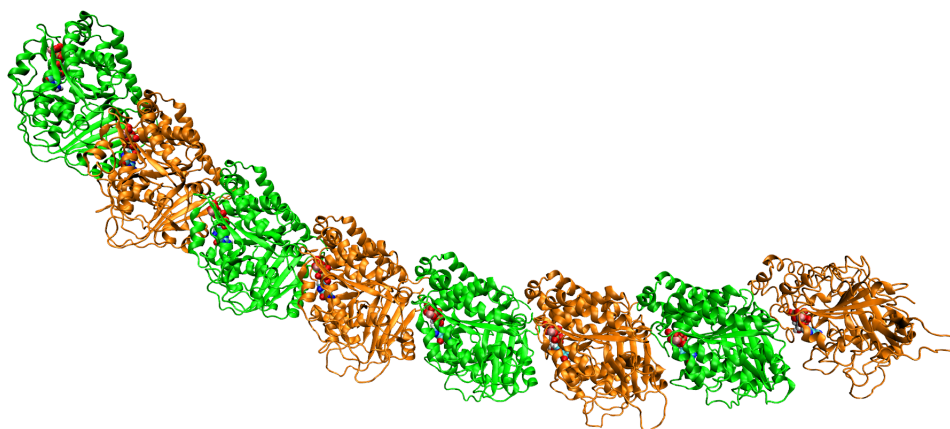


Figure 2.3: 4-dimer microtubule protofilament system (Tubulin from right to left: TA00, TB00, TA01, TB01, TA02, TB02, TA03, TB03)

2.2 Preparation for Simulation

After the structures were built as described in the previous sections, all of the systems followed the same procedure. The systems were prepared for MD simulations by submerging the protein into a water box (Figure 2.4). We used the explicit TIP3P water model as our solvent. We then neutralized the water box by adding Sodium (Na^+) and Chloride (Cl^-) ions randomly into the water box to bring the net charge of -72 for the 2-dimer system and -144 for the 4-dimer system to 0. While we could have added only Na^+ ions to the solution to bring the charge to 0, adding NaCl molecules to the system more accurately mimics the biological environment observed in a cell.

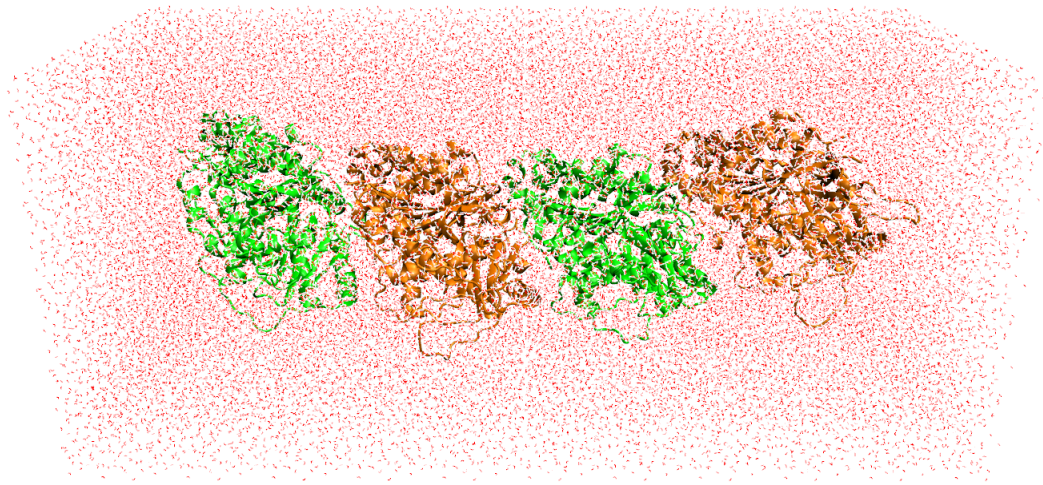


Figure 2.4: 2-dimer microtubule protofilament system submerged in water box

After neutralization was complete, we heated the entire system, water box and protein to 300 Kelvin (K). This process was performed in order to simulate how the protein would react in a room temperature environment. Once the system was heated there is excess energy in the system, meaning that the structure may not be in its lowest energy or equilibrium state. To address this problem, the protein was again “held” using a harmonic constraint, and was allowed to relax or equilibrate before beginning dynamic simulations. This is necessary as excess energy in the system can lead to the loss of integrity of the model, and is absolutely necessary to perform accurate MD simulations. We used this relaxed model to perform our MD simulations.

2.3 Molecular Dynamics Simulation

For our simulations, we utilized Texas A&M’s High Performance Research Computing Facilities, specifically their Ada and Terra clusters. We used CHARMM’s standard “Leapfrog Verlet” dynamic protocol, and also held the PF at constant temperature and pressure ensuring that the protein would remain at 300 K [10] [11] [12]. We also used

a Periodic Boundary Condition (PBC) to ensure that the filament would not become un-submerged from the water box. We took care to construct a large enough water box to accommodate the protein entering the box from the opposite side while avoiding self interactions. Initially, we ran a 1 ns simulation to ensure that our model would maintain its integrity, then continued the simulation in 5 ns intervals for a total simulation length of 400 ns for the 2-dimer systems and 210 ns for the 4-dimer simulations. We found these to be a sufficient starting simulation times as the different systems had time to show cyclic behavior which we could analyze to have significant results. However, these simulations only allow for us to make reserved predictions which can be supported by extending the simulations and running further analyses in the future.

2.4 Analysis of Simulation Trajectories

After completing the simulations, we combined all of the 5 ns trajectories of the individual atoms into one file for each system, and removed the water box to conserve system memory. We performed various analyses on the trajectories, including a center of mass, bending stiffness, and contact analysis which are detailed below.

2.4.1 Center of Mass Analysis

The center of mass analysis was used to develop a more complete understanding and “feel” of the protein. From the trajectories of the atoms, we calculated the coordinates for the center of mass (CM) of each tubulin using CHARMM. With the center of mass coordinates, we were able to calculate how much the CM position was varying throughout the simulation.

2.4.2 Bending Stiffness Analysis

The bending stiffness analysis used a method which was developed by Dr. Hwang and a former Ph.D. student Xiaojing Teng [13]. To calculate bending stiffness, a vector was

defined between the CM of the internal β -sheets of one tubulin, in the direction of the next adjacent tubulin's internal β -sheets. These specific coordinates were chosen because the internal β -sheets are quite immobile compared to the rest of the structure. Once this vector was defined, an entire orthonormal coordinate system was then generated [13]. This process was done for all tubulin pairs, for every frame of the simulation. With this data we were able to measure the differences between the angle of the vectors between tubulin for each frame. With these measurements we were able to calculate the principal axes of motion, bending stiffness along a major and minor axis as well as other mechanical properties of all the MT PF systems. Figure 2.5 shows the same structure seen in Figure 2.1, with the addition of the visualized triads.

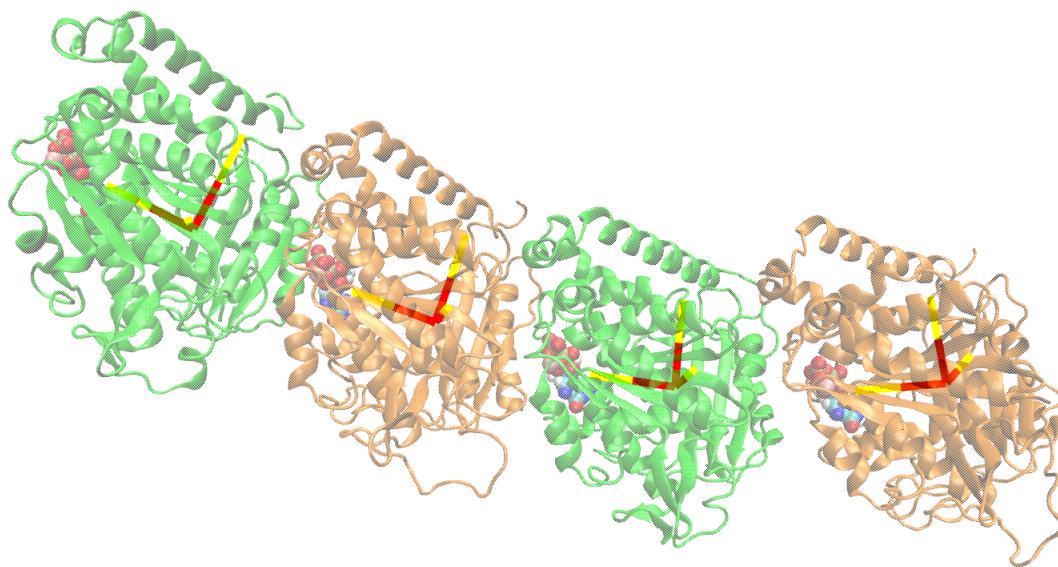


Figure 2.5: Triad analysis of 2-dimer microtubule protofilament system (Tubulin from right to left: TA00, TB00, TA01, TB01)

2.4.3 Contact Analysis

The contact analysis took each simulation frame by frame, and reported all polar and nonpolar contacts between two tubulin, between a nucleotide and the associated tubulin, as well as a nucleotide and the adjacent tubulin to determine if there were any polar or nonpolar contacts formed. We considered hydrogen bonds as polar contacts, and other various interactions (e.g. Van der Waals interactions) as nonpolar contacts. For this analysis, we specified two segments (i.e. two tubulin or a nucleotide and a tubulin). The CHARMM algorithm then went through each frame of the simulation and reported the polar or nonpolar contacts present, depending on which type of contact was specified in the input script. With this data we were able to run multiple programs written in C++ to analyze the data and return important findings.

The first C++ code collected all of the contacts formed (both polar and nonpolar) and calculated different properties. These properties included: how many contacts were formed in total, which frame in the simulation a contact either formed or broke, the percent occupancy of all contacts formed throughout the simulation, as well as other measurements. A second program was used to collect all high-occupancy contacts, which we defined as a contact present for 80.0% or more of the simulation, and return the amount as well as the specific amino acid residues involved in the contacts. From this point we were able to visualize the high occupancy contacts in VMD [14] [15] which can be seen in Figure 2.6. In the figure α -tubulin are highlighted in orange, β -tubulin are highlighted in green, atoms comprising the nucleotides are represented as spheres, nonpolar contacts between tubulin are in blue, and nonpolar contacts between the nucleotide and the associated tubulin are purple.

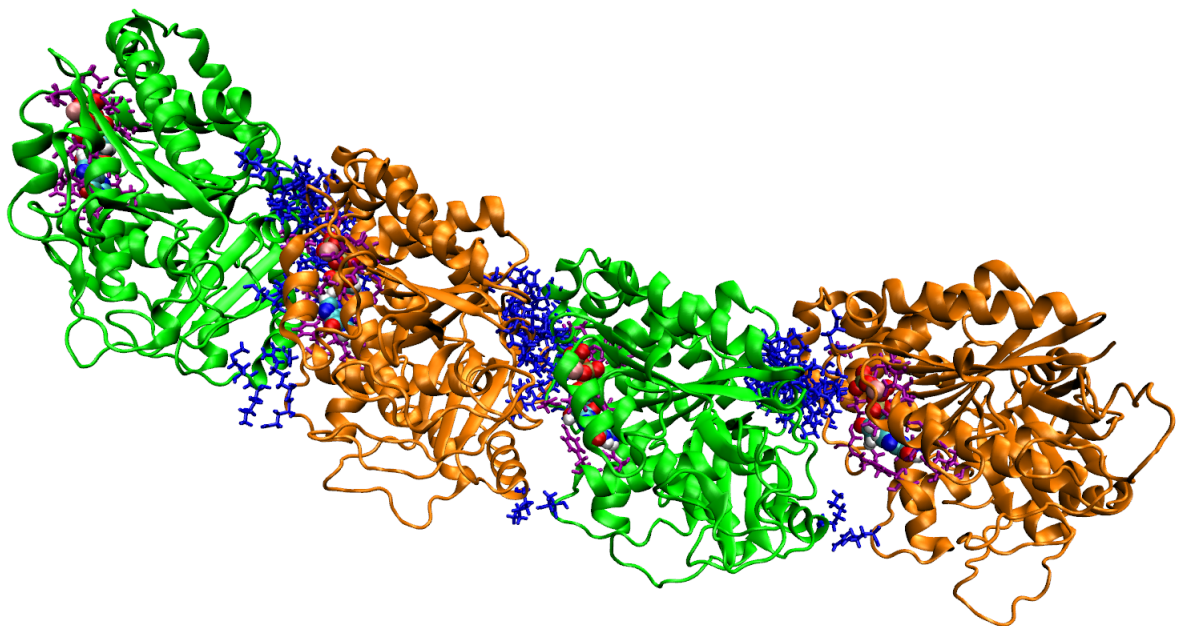


Figure 2.6: 2-dimer microtubule protofilament with high occupancy nonpolar contacts shown in a stick representation (Tubulin from right to left: TA00, TB00, TA01, TB01)

3. RESULTS AND DISCUSSION

From the analyses discussed above, we discovered several novel findings which are discussed below.

3.1 General Movement of Tubulin in a Microtubule Protofilament

From the CM analysis, we were able to visualize how each individual tubulin moved throughout the simulation. Figure 3.1 shows the CM position at each frame for all systems.

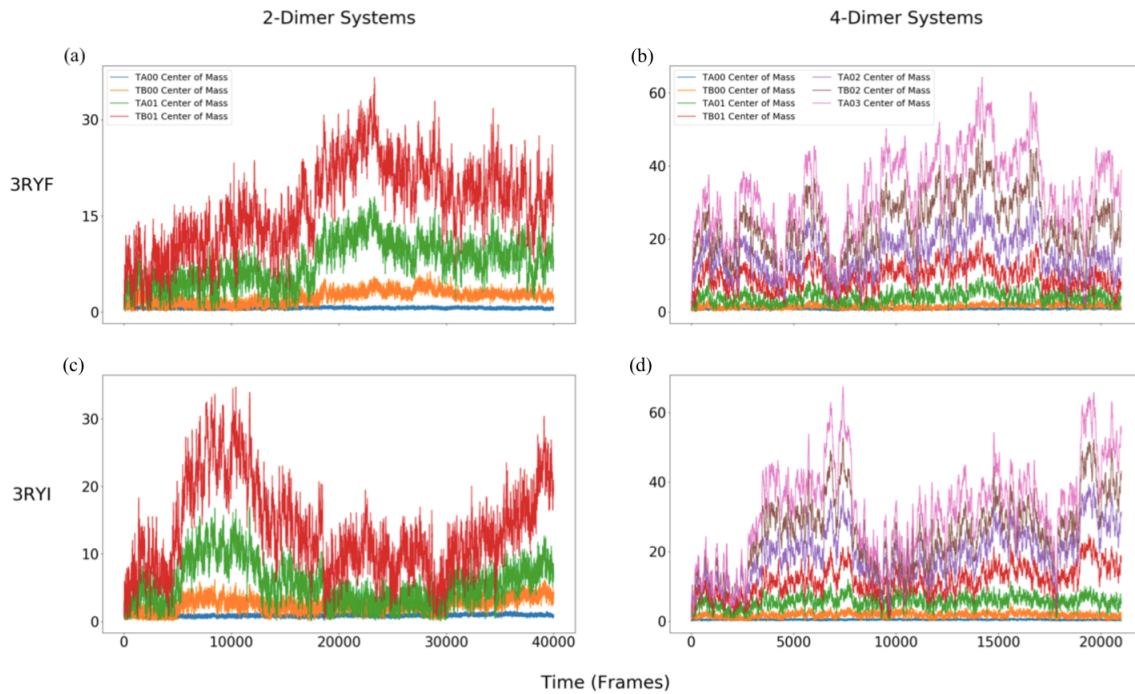


Figure 3.1: Center of mass position for all microtubule protofilament systems

From the plots seen in Figure 3.1, we were able to calculate the average and standard deviation of each tubulin's CM position. These results can be seen in Tables 3.1 & 3.2.

Table 3.1: 2-Dimer Systems Center of Mass Position Statistics.

2-Dimer Center of Mass Position Statistics			
Tubulin	<i>Statistical Measure</i>	3RYF	3RYI
TA00	<i>Average</i>	0.6174	0.8538
	<i>Standard Deviation</i>	0.1331	0.1776
TB00	<i>Average</i>	2.2587	2.3807
	<i>Standard Deviation</i>	1.0586	1.0421
TA01	<i>Average</i>	7.4929	5.5213
	<i>Standard Deviation</i>	3.4574	3.1524
TB01	<i>Average</i>	16.5678	13.5419
	<i>Standard Deviation</i>	6.5961	6.6116
End of Table 3.1			

Table 3.2: 4-Dimer Systems Center of Mass Position Statistics.

4-Dimer Center of Mass Position Statistics			
Tubulin	<i>Statistical Measure</i>	3RYF	3RYI
TA00	<i>Average</i>	0.8419	0.4569
	<i>Standard Deviation</i>	0.1637	0.1333
TB00	<i>Average</i>	1.5212	1.7611
	<i>Standard Deviation</i>	0.5709	0.7045
TA01	<i>Average</i>	3.8770	5.5267
	<i>Standard Deviation</i>	1.6862	1.7928
TB01	<i>Average</i>	9.3335	11.5663
	<i>Standard Deviation</i>	3.3853	4.1762

Table 3.2: Continued

Tubulin	<i>Statistical Measure</i>	3RYF	3RYI
TA02	<i>Average</i>	15.4813	19.0397
	<i>Standard Deviation</i>	5.6098	7.2363
TB02	<i>Average</i>	24.0763	25.3118
	<i>Standard Deviation</i>	8.1201	10.1814
TA03	<i>Average</i>	32.9529	32.4282
	<i>Standard Deviation</i>	11.0218	13.3281
TB03	<i>Average</i>	43.4873	42.0834
	<i>Standard Deviation</i>	13.5438	16.2737
End of Table 3.2			

While analyzing the data in Tables 3.1 & 3.2, both conformations have similar average values for the CM. This implies that both 3RYF and 3RYI have similar curvatures. From Table 3.1 it can be seen that the standard deviations of the CM positions are quite similar. However, looking at Table 3.2 it can be seen that in a larger, more mobile system, the standard deviation of the CM position for 3RYF is almost always lower than the standard deviation for 3RYI. This pattern can be more clearly seen as you move towards the free end of the PF (TB03). A lower standard deviation of the CM position implies that there is less change in the average position and therefore less overall motion. This decrease in motion seen in 3RYF compared to 3RYI implies that 3RYF is more stiff than 3RYI. Although 3RYF and 3RYI may have similar curvatures, 3RYF is more stiff which leads to the stability of the PF seen during rescue, whereas 3RYI is more flexible leading to the instability seen during catastrophe.

3.2 Mechanical Properties of Microtubule PFs

From our triad analysis detailed above, we were able to quantify several mechanical properties of the MT PFs including: the principal bending axes, bending stiffnesses with respect to the principal axes, average twist, twist stiffness, average extension, and extension stiffness. The report values can be seen in Tables 4.1 & 4.2. Unfortunately, based on the values reported in Tables 4.1 & 4.2, no definitive distinctions can be made. To further analyze the results, we measured the mechanical properties for the first half and second half of the simulations. Figures 3.2, 3.3, & 3.4 show the major and minor bending and twist stiffnesses for each tubulin pair for the first and second half of the simulations.

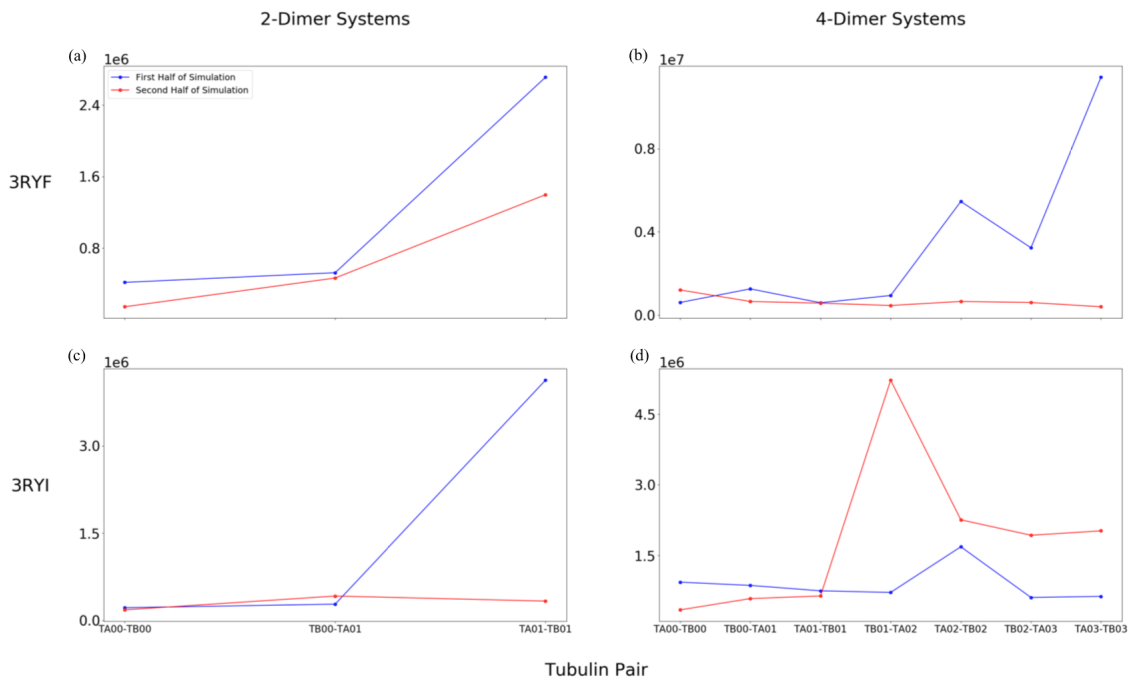


Figure 3.2: Major bending stiffness for the first and second half of the simulation for each pair of tubulin in all microtubule protofilament systems

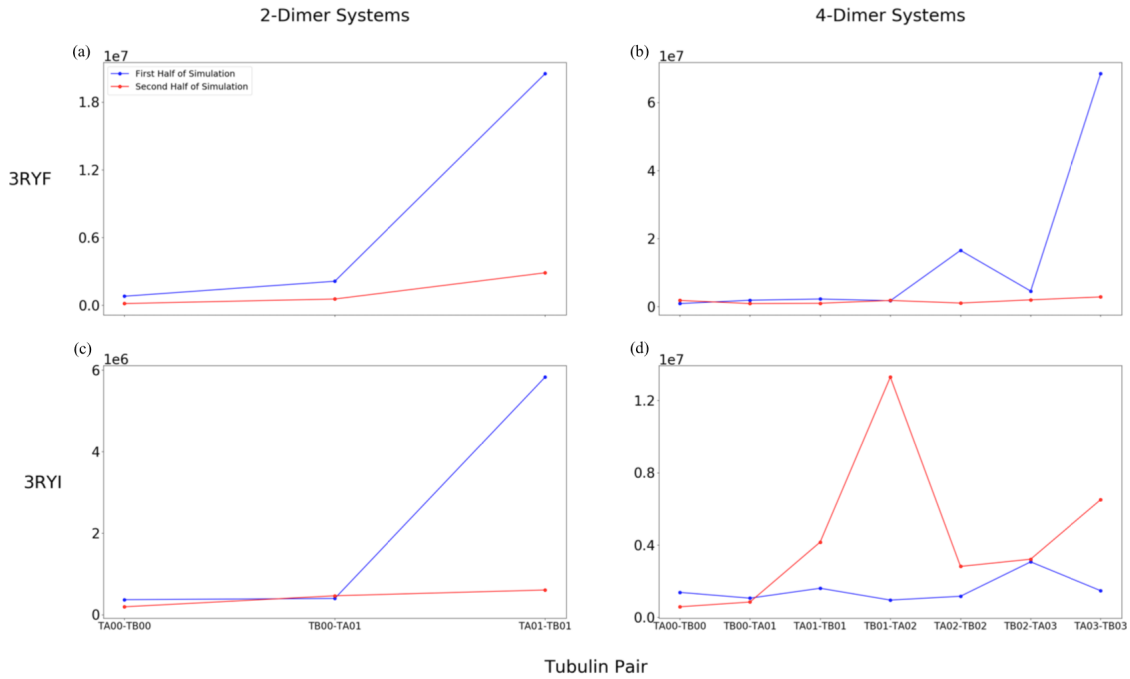


Figure 3.3: Minor bending stiffness for the first and second half of the simulation for each pair of tubulin in all microtubule protofilament systems

From these plots we think that with an extended simulation, the MT PF would begin behaving more naturally, therefore allowing us to analyze data which is more representative of a MT PF's native behavior. The simulation would need to be extended because there is time at the beginning of the simulation where the PF is still transitioning from the crystal structure it was imaged in, to the dynamic structure observed *in vivo*. This means some of the beginning frames must be removed, and leaves us with less frames than we would like for our analysis, so we must extend our simulations. However, based on Figures 3.2 & 3.3, we can make a few reserved predictions.

From the bending stiffness seen in Figures 3.2 a & c and Figures 3.3 a & c, 3RYF has a higher major bending stiffness compared to 3RYI. This supports the data found from the CM analysis. 3RYF moves relatively less than 3RYI, meaning 3RYF is more stiff

than 3RYI, which is supported by these plots. After extending the analysis it would be interesting to analyze the stiffness without the large jump in magnitude in the last tubulin pair analyzed. These same patterns hold true for the minor bending and twist stiffnesses as well.

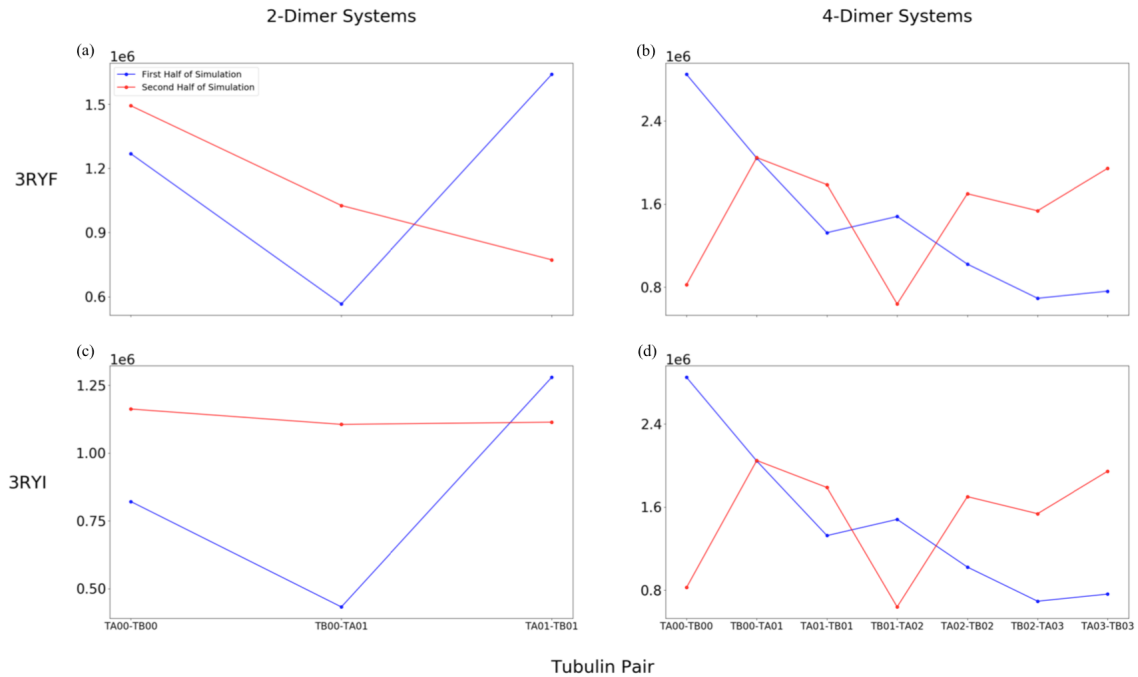


Figure 3.4: Twist bending stiffness for the first and second half of the simulation for each pair of tubulin in all microtubule protofilament systems

In Figures 3.2 b & d and Figures 3.3 b & d, we believe extending the simulations, and removing some initial frames from the analysis, would present the same patterns observed in the 2-dimer system for the 4-dimer system. However, we are limited by the length of the simulations, and cannot make any definitive claims about the properties observed.

3.3 Contacts Present in Microtubule PF Interfaces

From the contact analysis performed we found that in both the 2-dimer and 4-dimer systems 3RYF seemed to have contacts present in the interface located towards the luminal side of a MT. This can be seen by comparing Figures 3.5 b & d. In 3RYI the α -tubulin are bound to GTP and the β -tubulin are bound to GDP. This means that intra-dimer contacts of 3RYI should be similar to 3RYF, however, inter-dimer contacts should be different. As previously mentioned, in 3RYF there are contacts present in the interface located towards what would be the luminal side of a MT. These contacts were present in the entire 2-dimer structure of 3RYF, and only present in the similar intra-dimer interfaces of 3RYI. We believe that this is may be a phenomenon which leads to the increase in stability observed in 3RYF over 3RYI. However, these contacts were only present in the first half of the 4-dimer structure for 3RYF and in the first intra-dimer interface of 3RYI. We believe this is because as MT PFs grow in length they naturally curve more without having the lateral contacts formed when the PF is bound to a complete MT. This explains why the 2-dimer system displays these contacts throughout, and why the 4-dimer system loses these contacts as you move further along the PF.

In both conformations of the PF, polar contacts were centralized in the middle of the tubulin-tubulin interfaces, with nonpolar contacts located farther out from the center of the interface. We believe that this distribution of nonpolar contacts surrounding polar contacts occurs in an effort to protect the stronger more specific polar contacts from being interrupted by water molecules limiting relative twisting between tubulin. The contact analysis also revealed that there were similarities in the distribution of high occupancy contacts present in the two different conformations, seen in Figure 3.5.

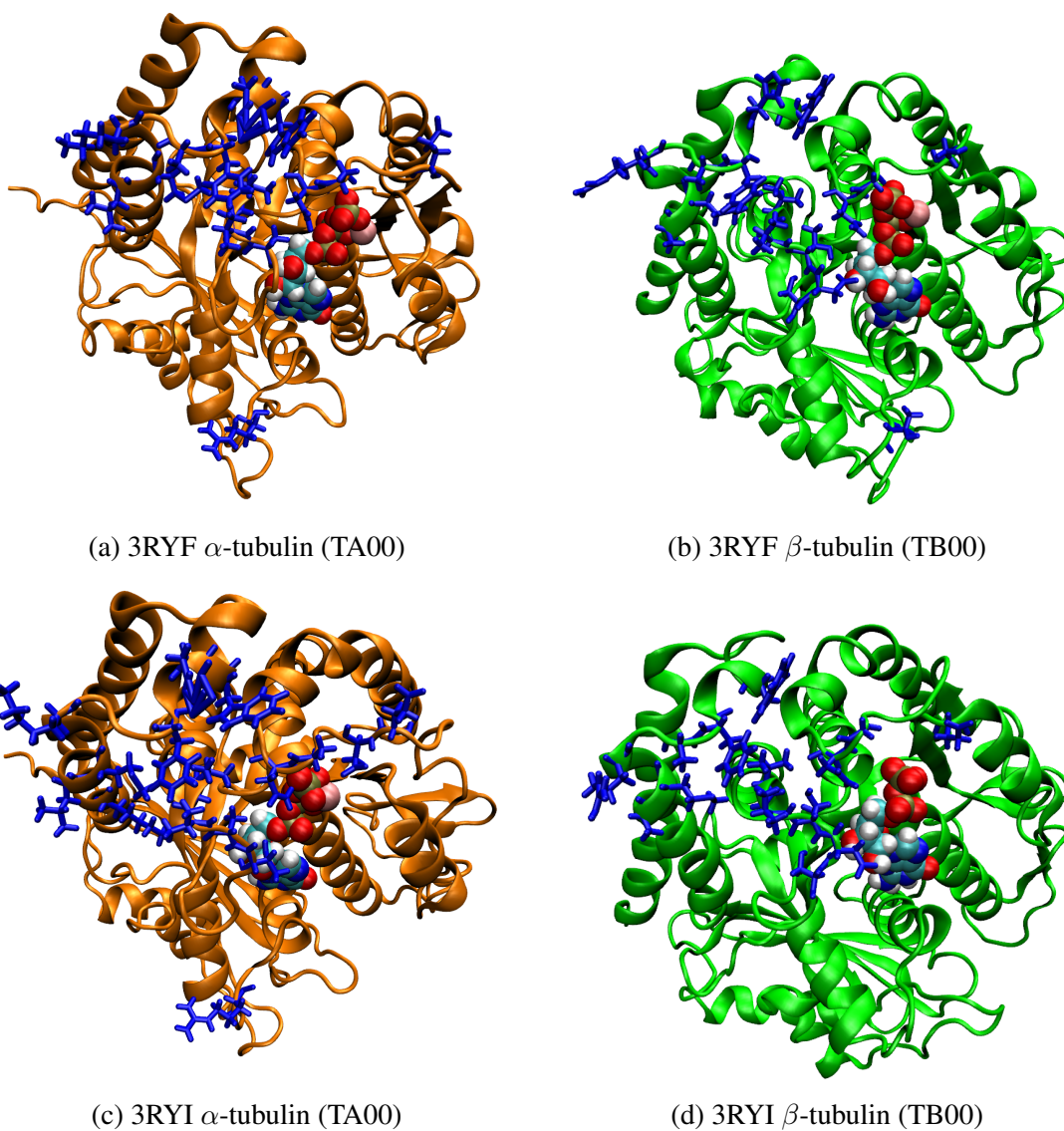


Figure 3.5: Axial View of the physical distribution of amino acid residues in first tubulin dimer of 3RYF & 3RYI, contacts are shown in stick representation

Additionally, many residues involved in polar and nonpolar contacts which had an occupancy above 90% were conserved in both conformations, this can be seen in Tables 4.3, 4.4, 4.5, & 4.6 (see appendix). While some of the contacts present in the two conformations were similar, there were also many slight differences found. For example, 3RYF

contained a contact between the amino acid residues of aspartate 98 and arginine 253, whereas 3RYI had a contact with the same aspartate 98 but with lysine 254. The contacts were both polar and located in the same general region of the interface, however, due to changes of the interface from the nucleotide present, the contact is altered slightly. We believe that some of these “shifted contacts” in 3RYI may be more weak and less stable than the corresponding contacts present in 3RYF.

We also found that 3RYF, contained nonpolar contacts between the phosphate tail of GTP and asparagine 101, alanine 99, and threonine 145. These amino acid residues seem to “protect” the nucleotide from hydrolysis by limiting water molecules from too easily accessing the nucleotide, therefore not allowing the instantaneous hydrolysis of GTP to GDP, this can be seen in Figure 3.6.

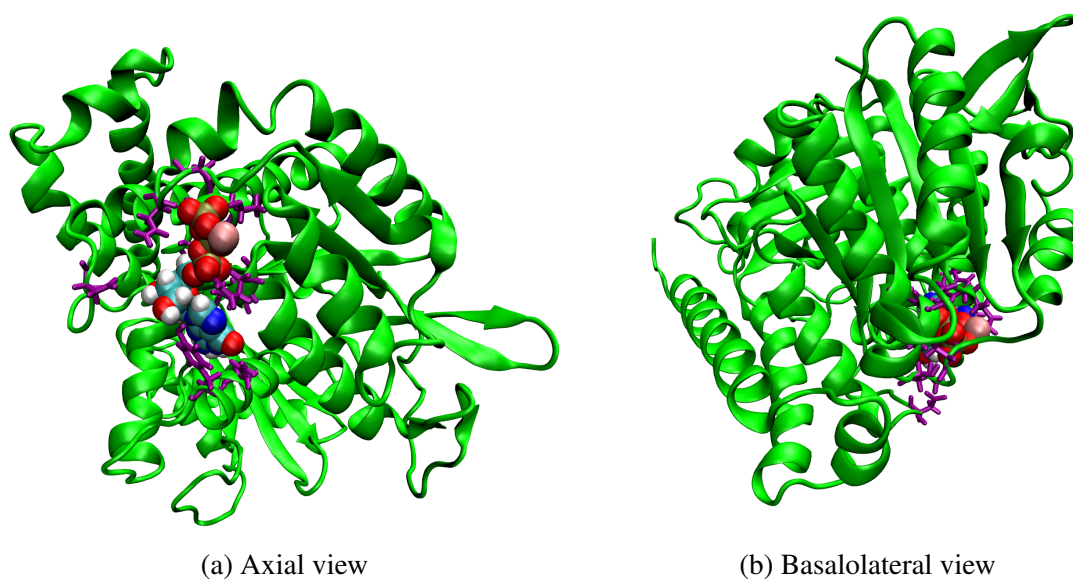


Figure 3.6: Residues protecting GTP from attack by water molecules shown in stick representation

4. CONCLUSION, APPLICATIONS, AND FUTURE DIRECTIONS

4.1 Conclusion

From this project we were able to accomplish several of our goals including: analyze the individual motion of tubulin in a 2-dimer and 4-dimer MT PF, quantify various mechanical properties of a 2-dimer and 4-dimer MT PF more accurately than which had been previously done, and establish the contacts present between tubulin of a MT PF. We have also learned that our simulations need to be extended in order to find more useful and representative results for the mechanical properties of all the MT PF systems.

4.2 Applications

From this project and future projects, we will have the ability to generate a coarse grained model of a MT PF. With this type of model we will be able to simulate much larger systems without exponentially increasing the computation time. These massive simulations can then answer further questions about the properties and behavior of MTs, as well as the effects of MT modifications, and associated proteins. From this project, as well as future projects, a better understanding of the complex properties and behaviors observed in MT PFs and MTs has the potential to lead to improvements in various disease treatments such as Cancer and Alzheimer's [1] [2].

4.3 Future Directions

Following this project we have identified several different avenues to pursue in the future. From the current project, we would like to: extend our simulations, study the contacts in more depth, study the effects of the specific contacts which were "shifted" as mentioned in **Chapter 3**, and describe a potential mechanism by which nucleotides (GTP

& GDP) control the dynamic behaviors observed in MTs. Another additional area we would like to pursue is researching different methods to decrease the computation time required for the simulation. In order for us to simulate the 2-dimer and 4-dimer systems for 400 and 210 ns, it required about 2 months of computation time for both systems, so 4 months in total. We are interested in looking into various ways to decrease this required computation time, such as implementing more robust GPU accelerated computing methods in tandem with more effective spatial decomposition methods to handle memory more efficiently to gain the ability to simulate larger systems.

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MECHANICAL PROPERTIES OF THE MICROTUBULE PROTOFILAMENT SYSTEMS

Table 4.1: Mechanical Properties of the 2-Dimer Microtubule Protofilament Systems.

2-Dimer MT Protofilament Mechanical Properties			
Tubulin Compared	Mechanical Property [<i>Unit</i>]	3RYF Magnitude	3RYI Magnitude
1 → 2	Major Kf [$pN \cdot \text{\AA}^2$]	$2.827 \cdot 10^5$	$1.925 \cdot 10^5$
	Minor Kf [$pN \cdot \text{\AA}^2$]	$6.529 \cdot 10^5$	$3.932 \cdot 10^5$
	Average Twistm [degrees]	-52.4992	-78.8542
	Twist Kf [$pN \cdot \text{\AA}^2$]	$1.031 \cdot 10^6$	$7.857 \cdot 10^5$
	Average Extension [\AA]	44.3248	43.4082
	Extension Kf [$pN/\text{\AA}$]	61.5905	204.0990
2 → 3	Major Kf [$pN \cdot \text{\AA}^2$]	$7.396 \cdot 10^5$	$2.936 \cdot 10^5$
	Minor Kf [$pN \cdot \text{\AA}^2$]	$1.926 \cdot 10^6$	$4.034 \cdot 10^5$
	Average Twistm [degrees]	-31.3051	-3.5806
	Twist Kf [$pN \cdot \text{\AA}^2$]	$6.458 \cdot 10^5$	$4.189 \cdot 10^5$
	Average Extension [\AA]	43.0475	43.2763
	Extension Kf [$pN/\text{\AA}$]	309.9571	152.2151

Table 4.1: Continued

Tubulin Compared	Mechanical Property [<i>Unit</i>]	3RYF Magnitude	3RYI Magnitude
3 → 4	Major Kf [$pN \cdot \text{\AA}^2$]	$2.663 \cdot 10^5$	$4.907 \cdot 10^6$
	Minor Kf [$pN \cdot \text{\AA}^2$]	$1.005 \cdot 10^7$	$5.969 \cdot 10^6$
	Average Twistm [degrees]	-78.0465	-9.4838
	Twist Kf [$pN \cdot \text{\AA}^2$]	$1.552 \cdot 10^6$	$1.336 \cdot 10^6$
	Average Extension [\AA]	43.4456	43.2790
	Extension Kf [$pN/\text{\AA}$]	491.6034	446.8574
End of Table 4.1			

Table 4.2: Mechanical Properties of the 4-Dimer Microtubule Protofilament Systems.

4-Dimer MT Protofilament Mechanical Properties			
Tubulin Compared	Mechanical Property [<i>Unit</i>]	3RYF Magnitude	3RYI Magnitude
1 → 2	Major Kf [$pN \cdot \text{\AA}^2$]	$3.675 \cdot 10^5$	$3.533 \cdot 10^5$
	Minor Kf [$pN \cdot \text{\AA}^2$]	$8.478 \cdot 10^5$	$1.015 \cdot 10^6$
	Average Twistm [degrees]	-69.6747	-35.5096
	Twist Kf [$pN \cdot \text{\AA}^2$]	$9.226 \cdot 10^5$	$1.840 \cdot 10^6$
	Average Extension [\AA]	44.0903	43.0281
	Extension Kf [$pN/\text{\AA}$]	231.5339	752.4633

Table 4.2: Continued

Tubulin Compared	Mechanical Property [<i>Unit</i>]	3RYF Magnitude	3RYI Magnitude
2 → 3	Major Kf [$pN \cdot \text{\AA}^2$]	$8.037 \cdot 10^5$	$7.307 \cdot 10^5$
	Minor Kf [$pN \cdot \text{\AA}^2$]	$1.059 \cdot 10^6$	$1.269 \cdot 10^6$
	Average Twistm [degrees]	-18.9700	-53.3611
	Twist Kf [$pN \cdot \text{\AA}^2$]	$1.238 \cdot 10^6$	$1.245 \cdot 10^6$
	Average Extension [\AA]	43.2797	43.6684
	Extension Kf [$pN/\text{\AA}$]	417.6528	165.6772
3 → 4	Major Kf [$pN \cdot \text{\AA}^2$]	$4.865 \cdot 10^5$	$1.232 \cdot 10^6$
	Minor Kf [$pN \cdot \text{\AA}^2$]	$1.174 \cdot 10^6$	$2.596 \cdot 10^6$
	Average Twistm [degrees]	-77.8632	-33.3405
	Twist Kf [$pN \cdot \text{\AA}^2$]	$1.257 \cdot 10^6$	$7.122 \cdot 10^5$
	Average Extension [\AA]	44.4319	44.3402
	Extension Kf [$pN/\text{\AA}$]	146.4000	165.6772
4 → 5	Major Kf [$pN \cdot \text{\AA}^2$]	$2.735 \cdot 10^5$	$1.100 \cdot 10^6$
	Minor Kf [$pN \cdot \text{\AA}^2$]	$9.822 \cdot 10^5$	$1.207 \cdot 10^6$
	Average Twistm [degrees]	-80.6750	-64.1595
	Twist Kf [$pN \cdot \text{\AA}^2$]	$5.468 \cdot 10^5$	$1.081 \cdot 10^6$
	Average Extension [\AA]	43.7137	43.6563
	Extension Kf [$pN/\text{\AA}$]	97.5755	243.2915

Table 4.2: Continued

Tubulin Compared	Mechanical Property [<i>Unit</i>]	3RYF Magnitude	3RYI Magnitude
5 → 6	Major Kf [$pN \cdot \text{\AA}^2$]	$1.036 \cdot 10^6$	$1.965 \cdot 10^6$
	Minor Kf [$pN \cdot \text{\AA}^2$]	$3.237 \cdot 10^6$	$1.420 \cdot 10^6$
	Average Twistm [degrees]	-63.5055	2.8270
	Twist Kf [$pN \cdot \text{\AA}^2$]	$7.732 \cdot 10^5$	$1.192 \cdot 10^6$
	Average Extension [\AA]	43.8363	42.5272
	Extension Kf [$pN/\text{\AA}$]	136.2962	322.1116
6 → 7	Major Kf [$pN \cdot \text{\AA}^2$]	$3.945 \cdot 10^5$	$3.928 \cdot 10^5$
	Minor Kf [$pN \cdot \text{\AA}^2$]	$3.047 \cdot 10^6$	$3.420 \cdot 10^6$
	Average Twistm [degrees]	-30.5846	-43.0967
	Twist Kf [$pN \cdot \text{\AA}^2$]	$4.196 \cdot 10^5$	$5.697 \cdot 10^5$
	Average Extension [\AA]	43.7499	43.6818
	Extension Kf [$pN/\text{\AA}$]	333.5413	310.5092
7 → 8	Major Kf [$pN \cdot \text{\AA}^2$]	$2.237 \cdot 10^6$	$7.928 \cdot 10^5$
	Minor Kf [$pN \cdot \text{\AA}^2$]	$1.101 \cdot 10^7$	$1.719 \cdot 10^6$
	Average Twistm [degrees]	-66.8805	-80.9410
	Twist Kf [$pN \cdot \text{\AA}^2$]	$8.120 \cdot 10^5$	$3.833 \cdot 10^5$
	Average Extension [\AA]	43.6565	43.8037
	Extension Kf [$pN/\text{\AA}$]	234.6173	199.3189
End of Table 4.2			

LIST OF CONTACTS PRESENT BETWEEN TUBULIN IN THE MICROTUBULE PROTOFILAMENT SYSTEMS

Table 4.3: Contacts Present in 3RYF 2-Dimer Microtubule Protofilament.

Contacts Present in 3RYF 2-Dimer System			
Contact Type	Contact	Domain	% Occupancy
Polar	PHE 404 - PRO 261	TA00 - TB00	99.542
Polar	GLU 97 - ARG 164	TA00 - TB00	94.787
Polar	VAL 181 - ASN 258	TA00 - TB00	82.107
Polar	PHE 404 - PRO 261	TB00 - TA01	93.790
Polar	THR 180 - ASN 258	TB00 - TA01	92.405
Polar	ARG 401 - TYR 262	TB00 - TA01	86.005
Polar	PHE 404 - PRO 261	TA01 - TB01	99.775
Polar	ASP 98 - LYS 254	TA01 - TB01	99.612
Polar	ARG 221 - ASP 329	TA01 - TB01	98.965
Polar	GLU 97 - ARG 164	TA01 - TB01	96.370
Polar	GTP 1 - THR 145	GTP - TA00	99.995
Polar	GTP 1 - ASN 228	GTP - TA00	99.995
Polar	GTP 1 - GLN 11	GTP - TA00	99.770
Polar	GTP 1 - ALA 12	GTP - TA00	99.147
Polar	GTP 1 - GLY 146	GTP - TA00	98.225
Polar	GTP 1 - ASN 206	GTP - TA00	97.742
Polar	GTP 2 - THR 145	GTP - TB00	100.000
Polar	GTP 2 - ASN 101	GTP - TB00	99.947

Table 4.3: Continued

Contact Type	Contact	Domain	% Occupancy
Polar	GTP 2 - ASN 228	GTP - TB00	99.922
Polar	GTP 2 - CYS 12	GTP - TB00	98.775
Polar	GTP 2 - GLY 146	GTP - TB00	92.240
Polar	GTP 2 - GLY 144	GTP - TB00	88.175
Polar	GTP 3 - ASN 101	GTP - TA01	100.000
Polar	GTP 3 - THR 145	GTP - TA01	100.000
Polar	GTP 3 - ASN 228	GTP - TA01	99.982
Polar	GTP 3 - GLY 144	GTP - TA01	99.935
Polar	GTP 3 - GLY 146	GTP - TA01	99.867
Polar	GTP 3 - GLN 11	GTP - TA01	99.647
Polar	GTP 3 - ALA 12	GTP - TA01	99.572
Polar	GTP 3 - ASN 206	GTP - TA01	93.575
Polar	GTP 3 - THR 179	GTP - TA01	82.092
Polar	GTP 4 - THR 145	GTP - TB01	99.997
Polar	GTP 4 - ASN 228	GTP - TB01	99.995
Polar	GTP 4 - CYS 12	GTP - TB01	98.942
Polar	GTP 4 - ASN 101	GTP - TB01	97.910
Polar	GTP 4 - GLY 146	GTP - TB01	89.875
Polar	GTP 4 - ASN 206	GTP - TB01	87.352
Polar	GTP 4 - TYR 224	GTP - TB01	82.210
Nonpolar	PHE 404 - PRO 261	TA00 - TB00	100.000
Nonpolar	VAL 181 - ASN 258	TA00 - TB00	99.927
Nonpolar	TRP 407 - VAL 260	TA00 - TB00	99.842

Table 4.3: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	ALA 180 - ASN 258	TA00 - TB00	99.292
Nonpolar	LYS 401 - PHE 262	TA00 - TB00	98.642
Nonpolar	HIS 406 - PRO 263	TA00 - TB00	98.442
Nonpolar	ALA 100 - LYS 254	TA00 - TB00	98.217
Nonpolar	ASN 101 - LYS 254	TA00 - TB00	97.910
Nonpolar	ALA 100 - ARG 253	TA00 - TB00	97.840
Nonpolar	PHE 404 - ILE 0347	TA00 - TB00	97.705
Nonpolar	GLU 097 - MET 1	TA00 - TB00	96.002
Nonpolar	ARG 221 - LYS 326	TA00 - TB00	95.200
Nonpolar	GLU 97 - ARG 164	TA00 - TB00	95.160
Nonpolar	LEU 397 - TRP 346	TA00 - TB00	95.092
Nonpolar	TRP 407 - VAL 257	TA00 - TB00	90.870
Nonpolar	VAL 182 - VAL 257	TA00 - TB00	89.355
Nonpolar	LEU 397 - PRO 348	TA00 - TB00	89.265
Nonpolar	PHE 404 - VAL 257	TA00 - TB00	86.330
Nonpolar	MET 398 - PRO 348	TA00 - TB00	84.945
Nonpolar	TRP 407 - ALA 256	TA00 - TB00	83.907
Nonpolar	ALA 403 - PRO 261	TA00 - TB00	83.435
Nonpolar	PHE 404 - PRO 261	TB00 - TA01	100.000
Nonpolar	THR 180 - ASN 258	TB00 - TA01	99.880
Nonpolar	ASP 179 - LYS 352	TB00 - TA01	99.622
Nonpolar	TRP 407 - GLN 256	TB00 - TA01	99.392
Nonpolar	TRP 407 - VAL 260	TB00 - TA01	97.715

Table 4.3: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	VAL 181 - PRO 348	TB00 - TA01	95.192
Nonpolar	GLY 100 - THR 253	TB00 - TA01	94.782
Nonpolar	SER 178 - GLY 350	TB00 - TA01	94.372
Nonpolar	ALA 397 - TRP 346	TB00 - TA01	93.477
Nonpolar	ARG 401 - TYR 262	TB00 - TA01	93.345
Nonpolar	VAL 182 - THR 257	TB00 - TA01	93.095
Nonpolar	TRP 407 - ASP 199	TB00 - TA01	92.352
Nonpolar	THR 221 - LYS 326	TB00 - TA01	92.140
Nonpolar	HIS 406 - PRO 263	TB00 - TA01	91.852
Nonpolar	ASN 101 - THR 257	TB00 - TA01	91.787
Nonpolar	ASN 101 - GLU 254	TB00 - TA01	91.607
Nonpolar	TRP 407 - THR 257	TB00 - TA01	90.927
Nonpolar	GLY 100 - THR 257	TB00 - TA01	89.097
Nonpolar	ALA 403 - TRP 346	TB00 - TA01	88.870
Nonpolar	SER 97 - ARG 002	TB00 - TA01	87.540
Nonpolar	MET 398 - TRP 346	TB00 - TA01	86.122
Nonpolar	ASP 179 - PHE 351	TB00 - TA01	85.795
Nonpolar	MET 398 - PRO 348	TB00 - TA01	85.417
Nonpolar	GLY 100 - GLU 254	TB00 - TA01	85.275
Nonpolar	VAL 181 - ASN 258	TB00 - TA01	83.832
Nonpolar	PHE 404 - PRO 261	TA01 - TB01	100.000
Nonpolar	TRP 407 - VAL 260	TA01 - TB01	99.985
Nonpolar	ALA 100 - LYS 254	TA01 - TB01	99.985

Table 4.3: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	ASP 98 - LYS 254	TA01 - TB01	99.950
Nonpolar	ALA 180 - ASN 258	TA01 - TB01	99.890
Nonpolar	PHE 404 - ILE 347	TA01 - TB01	99.777
Nonpolar	ARG 221 - ASP 329	TA01 - TB01	99.452
Nonpolar	LEU 397 - TRP 346	TA01 - TB01	99.210
Nonpolar	ASN 101 - LYS 254	TA01 - TB01	99.202
Nonpolar	VAL 181 - ASN 258	TA01 - TB01	99.017
Nonpolar	TRP 407 - ALA 256	TA01 - TB01	98.565
Nonpolar	LYS 394 - PRO 348	TA01 - TB01	98.562
Nonpolar	THR 179 - LEU 248	TA01 - TB01	97.800
Nonpolar	HIS 406 - PRO 263	TA01 - TB01	97.780
Nonpolar	LYS 401 - PHE 262	TA01 - TB01	97.682
Nonpolar	ALA 100 - ARG 253	TA01 - TB01	97.157
Nonpolar	GLU 97 - ARG 164	TA01 - TB01	96.840
Nonpolar	ARG 221 - LYS 326	TA01 - TB01	96.517
Nonpolar	MET 398 - PRO 348	TA01 - TB01	96.042
Nonpolar	SER 178 - LYS 352	TA01 - TB01	95.502
Nonpolar	TRP 407 - VAL 257	TA01 - TB01	94.972
Nonpolar	MET 398 - ILE 347	TA01 - TB01	93.927
Nonpolar	GLU 220 - LYS 326	TA01 - TB01	93.052
Nonpolar	HIS 406 - VAL 260	TA01 - TB01	91.995
Nonpolar	PHE 404 - VAL 257	TA01 - TB01	90.847
Nonpolar	PRO 175 - ASN 349	TA01 - TB01	90.037

Table 4.3: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	VAL 181 - ILE 347	TA01 - TB01	89.512
Nonpolar	ARG 221 - MET 325	TA01 - TB01	87.632
Nonpolar	VAL 182 - VAL 257	TA01 - TB01	84.470
Nonpolar	VAL 181 - ASN 350	TA01 - TB01	82.345
Nonpolar	ALA 100 - VAL 257	TA01 - TB01	82.102
Nonpolar	LEU 397 - PRO 348	TA01 - TB01	81.940
Nonpolar	GTP 1 - ASN 228	GTP - TA00	100.000
Nonpolar	GTP 1 - GLY 146	GTP - TA00	100.000
Nonpolar	GTP 1 - THR 145	GTP - TA00	100.000
Nonpolar	GTP 1 - ALA 12	GTP - TA00	100.000
Nonpolar	GTP 1 - GLN 11	GTP - TA00	100.000
Nonpolar	GTP 1 - GLY 143	GTP - TA00	99.982
Nonpolar	GTP 1 - ASN 206	GTP - TA00	99.932
Nonpolar	GTP 1 - ASP 69	GTP - TA00	99.782
Nonpolar	GTP 1 - SER 140	GTP - TA00	99.652
Nonpolar	GTP 1 - GLU 183	GTP - TA00	98.347
Nonpolar	GTP 1 - TYR 224	GTP - TA00	97.760
Nonpolar	GTP 1 - GLY 10	GTP - TA00	96.037
Nonpolar	GTP 1 - SER 178	GTP - TA00	93.992
Nonpolar	GTP 1 - GLY 144	GTP - TA00	93.882
Nonpolar	GTP 1 - VAL 177	GTP - TA00	90.872
Nonpolar	GTP 1 - GLN 15	GTP - TA00	86.087
Nonpolar	GTP 1 - ILE 231	GTP - TA00	81.350

Table 4.3: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GTP 1 - ALA 99	GTP - TA00	80.405
Nonpolar	GTP 2 - THR 145	GTP - TB00	100.000
Nonpolar	GTP 2 - GLY 143	GTP - TB00	100.000
Nonpolar	GTP 2 - ASN 101	GTP - TB00	100.000
Nonpolar	GTP 2 - CYS 12	GTP - TB00	100.000
Nonpolar	GTP 2 - ASN 228	GTP - TB00	99.997
Nonpolar	GTP 2 - GLY 146	GTP - TB00	99.997
Nonpolar	GTP 2 - GLN 11	GTP - TB00	99.957
Nonpolar	GTP 2 - GLY 144	GTP - TB00	99.892
Nonpolar	GTP 2 - ALA 99	GTP - TB00	99.775
Nonpolar	GTP 2 - TYR 224	GTP - TB00	95.797
Nonpolar	GTP 2 - ASP 179	GTP - TB00	94.890
Nonpolar	GTP 3 - ASN 228	GTP - TB01	100.000
Nonpolar	GTP 3 - GLY 146	GTP - TB01	100.000
Nonpolar	GTP 3 - THR 145	GTP - TB01	100.000
Nonpolar	GTP 3 - GLY 144	GTP - TB01	100.000
Nonpolar	GTP 3 - GLY 143	GTP - TB01	100.000
Nonpolar	GTP 3 - ASN 101	GTP - TB01	100.000
Nonpolar	GTP 3 - ALA 12	GTP - TB01	100.000
Nonpolar	GTP 3 - GLN 11	GTP - TB01	100.000
Nonpolar	GTP 3 - SER 140	GTP - TB01	99.785
Nonpolar	GTP 3 - ASN 206	GTP - TB01	99.777
Nonpolar	GTP 3 - ASP 69	GTP - TB01	99.720

Table 4.3: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GTP 3 - GLU 183	GTP - TB01	99.545
Nonpolar	GTP 3 - THR 179	GTP - TB01	99.387
Nonpolar	GTP 3 - TYR 224	GTP - TB01	96.340
Nonpolar	GTP 3 - GLY 10	GTP - TB01	92.635
Nonpolar	GTP 3 - ALA 99	GTP - TB01	83.975
Nonpolar	GTP 3 - VAL 177	GTP - TB01	81.040
End of Table 4.3			

Table 4.4: Contacts Present in 3RYI 2-Dimer Microtubule Protofilament.

Contacts Present in 3RYI 2-Dimer System			
Contact Type	Contact	Domain	% Occupancy
Polar	PHE 404 - PRO 261	TA00 - TB00	99.432
Polar	GLU 97 - ARG 253	TA00 - TB00	93.760
Polar	GLU 97 - ARG 164	TA00 - TB00	93.315
Polar	ARG 221 - GLU 330	TA00 - TB00	83.270
Polar	ASP 98 - LYS 254	TA00 - TB00	81.322
Polar	GLU 71 - ARG 2	TB00 - TA01	97.422
Polar	PHE 404 - PRO 261	TB00 - TA01	93.507
Polar	ASN 101 - ASN 258	TB00 - TA01	92.197
Polar	GLU 97 - ARG 164	TA01 - TB01	99.712
Polar	PHE 404 - PRO 261	TA01 - TB01	99.595
Polar	ARG 221 - ASP 329	TA01 - TB01	99.145
Polar	GLU 71 - MET 1	TA01 - TB01	89.180

Table 4.4: Continued

Contact Type	Contact	Domain	% Occupancy
Polar	ASP 98 - LYS 254	TA01 - TB01	83.922
Polar	GTP 1 - THR 145	GTP - TA00	100.000
Polar	GTP 1 - ASN 228	GTP - TA00	99.995
Polar	GTP 1 - ALA 12	GTP - TA00	99.500
Polar	GTP 1 - GLN 11	GTP - TA00	99.360
Polar	GTP 1 - GLY 146	GTP - TA00	98.175
Polar	GTP 1 - ASN 206	GTP - TA00	94.430
Polar	GTP 1 - GLY 144	GTP - TA00	84.797
Polar	GDP 1 - ASN 228	GDP - TB00	99.592
Polar	GTP 2 - THR 145	GTP - TA01	100.000
Polar	GTP 2 - GLY 144	GTP - TA01	99.970
Polar	GTP 2 - ASN 228	GTP - TA01	99.970
Polar	GTP 2 - ASN 101	GTP - TA01	99.955
Polar	GTP 2 - GLY 146	GTP - TA01	99.902
Polar	GTP 2 - GLN 11	GTP - TA01	99.265
Polar	GTP 2 - ALA 12	GTP - TA01	99.077
Polar	GTP 2 - ASN 206	GTP - TA01	86.755
Polar	GTP 2 - THR 179	GTP - TA01	80.775
Polar	GDP 2 - ASN 228	GDP - TB01	99.965
Polar	GDP 2 - ASN 206	GDP - TB01	96.505
Polar	GDP 2 - TYR 224	GDP - TB01	91.882
Nonpolar	PHE 404 - PRO 261	TA00 - TB00	100.000
Nonpolar	ALA 100 - LYS 254	TA00 - TB00	99.982

Table 4.4: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	TRP 407 - VAL 260	TA00 - TB00	99.825
Nonpolar	PHE 404 - ILE 347	TA00 - TB00	99.182
Nonpolar	THR 179 - LEU 248	TA00 - TB00	98.630
Nonpolar	ASP 98 - LYS 254	TA00 - TB00	98.547
Nonpolar	ARG 221 - LYS 326	TA00 - TB00	98.115
Nonpolar	HIS 406 - PRO 263	TA00 - TB00	98.040
Nonpolar	TRP 407 - ALA 256	TA00 - TB00	98.005
Nonpolar	LEU 397 - TRP 346	TA00 - TB00	97.875
Nonpolar	GLU 97 - ARG 253	TA00 - TB00	96.935
Nonpolar	VAL 181 - ASN 258	TA00 - TB00	96.835
Nonpolar	ALA 100 - ARG 253	TA00 - TB00	96.015
Nonpolar	LYS 401 - PHE 262	TA00 - TB00	95.982
Nonpolar	MET 398 - PRO 348	TA00 - TB00	95.405
Nonpolar	GLU 97 - ARG 164	TA00 - TB00	94.845
Nonpolar	ASN 101 - LYS 254	TA00 - TB00	93.482
Nonpolar	TRP 407 - VAL 257	TA00 - TB00	93.417
Nonpolar	VAL 182 - VAL 257	TA00 - TB00	92.240
Nonpolar	ALA 180 - ASN 258	TA00 - TB00	91.572
Nonpolar	GLU 97 - MET 1	TA00 - TB00	90.647
Nonpolar	PHE 404 - VAL 257	TA00 - TB00	89.802
Nonpolar	LEU 397 - PRO 348	TA00 - TB00	89.555
Nonpolar	LYS 401 - THR 439	TA00 - TB00	88.547
Nonpolar	LYS 401 - TRP 346	TA00 - TB00	86.755

Table 4.4: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	HIS 406 - VAL 260	TA00 - TB00	86.342
Nonpolar	ASN 101 - VAL 257	TA00 - TB00	85.670
Nonpolar	ARG 221 - GLU 330	TA00 - TB00	83.792
Nonpolar	LYS 401 - ALA 438	TA00 - TB00	83.412
Nonpolar	LYS 394 - PRO 348	TA00 - TB00	82.927
Nonpolar	VAL 181 - ILE 347	TA00 - TB00	81.935
Nonpolar	MET 398 - ILE 347	TA00 - TB00	81.242
Nonpolar	ARG 221 - GLU 327	TA00 - TB00	81.207
Nonpolar	PHE 404 - PRO 261	TB00 - TA01	99.997
Nonpolar	ASN 101 - ASN 258	TB00 - TA01	99.155
Nonpolar	THR 180 - ASN 258	TB00 - TA01	98.827
Nonpolar	ASN 101 - LYS 352	TB00 - TA01	98.697
Nonpolar	TRP 407 - VAL 260	TB00 - TA01	98.547
Nonpolar	ASP 179 - LYS 352	TB00 - TA01	98.020
Nonpolar	GLU 71 - ARG 2	TB00 - TA01	97.510
Nonpolar	ASN 101 - GLU 254	TB00 - TA01	96.922
Nonpolar	TRP 407 - GLN 256	TB00 - TA01	96.885
Nonpolar	GLY 100 - GLU 254	TB00 - TA01	95.977
Nonpolar	VAL 181 - PRO 348	TB00 - TA01	94.167
Nonpolar	ALA 397 - TRP 346	TB00 - TA01	93.867
Nonpolar	VAL 181 - ASN 258	TB00 - TA01	93.570
Nonpolar	GLY 100 - THR 253	TB00 - TA01	93.540
Nonpolar	SER 178 - GLY 350	TB00 - TA01	92.707

Table 4.4: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	ALA 403 - TRP 346	TB00 - TA01	90.392
Nonpolar	MET 398 - PRO 348	TB00 - TA01	90.357
Nonpolar	VAL 182 - THR 257	TB00 - TA01	90.355
Nonpolar	TRP 407 - THR 257	TB00 - TA01	88.875
Nonpolar	MET 398 - TRP 346	TB00 - TA01	87.962
Nonpolar	GLY 100 - THR 257	TB00 - TA01	86.525
Nonpolar	ALA 403 - TYR 262	TB00 - TA01	84.345
Nonpolar	ALA 403 - PRO 261	TB00 - TA01	84.140
Nonpolar	TRP 407 - ASP 199	TB00 - TA01	81.310
Nonpolar	ARG 401 - TRP 346	TB00 - TA01	81.170
Nonpolar	PHE 404 - PRO 261	TA01 - TB01	100.000
Nonpolar	ALA 100 - LYS 254	TA01 - TB01	99.997
Nonpolar	TRP 407 - VAL 260	TA01 - TB01	99.947
Nonpolar	GLU 97 - ARG 164	TA01 - TB01	99.802
Nonpolar	ALA 180 - ASN 258	TA01 - TB01	99.687
Nonpolar	ARG 221 - ASP 329	TA01 - TB01	99.590
Nonpolar	PHE 404 - ILE 347	TA01 - TB01	99.072
Nonpolar	LYS 401 - PHE 262	TA01 - TB01	99.060
Nonpolar	ALA 100 - ARG 253	TA01 - TB01	98.522
Nonpolar	THR 179 - LEU 248	TA01 - TB01	98.477
Nonpolar	VAL 181 - ASN 258	TA01 - TB01	98.357
Nonpolar	TRP 407 - ALA 256	TA01 - TB01	97.967
Nonpolar	HIS 406 - PRO 263	TA01 - TB01	97.960

Table 4.4: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	ASN 101 - LYS 254	TA01 - TB01	97.837
Nonpolar	ASP 98 - LYS 254	TA01 - TB01	96.912
Nonpolar	ARG 221 - LYS 326	TA01 - TB01	96.802
Nonpolar	GLU 71 - MET 1	TA01 - TB01	95.210
Nonpolar	MET 398 - PRO 348	TA01 - TB01	94.917
Nonpolar	LEU 397 - TRP 346	TA01 - TB01	94.900
Nonpolar	TRP 407 - VAL 257	TA01 - TB01	94.275
Nonpolar	ASP 98 - MET 1	TA01 - TB01	92.540
Nonpolar	ARG 221 - MET 325	TA01 - TB01	91.757
Nonpolar	GLU 97 - MET 1	TA01 - TB01	89.245
Nonpolar	THR 179 - ASN 258	TA01 - TB01	89.152
Nonpolar	GLU 220 - LYS 326	TA01 - TB01	87.327
Nonpolar	HIS 406 - VAL 260	TA01 - TB01	86.857
Nonpolar	VAL 181 - ILE 347	TA01 - TB01	86.757
Nonpolar	LEU 397 - PRO 348	TA01 - TB01	85.632
Nonpolar	ALA 403 - PRO 261	TA01 - TB01	85.605
Nonpolar	PHE 404 - VAL 257	TA01 - TB01	84.925
Nonpolar	LYS 401 - TRP 346	TA01 - TB01	83.435
Nonpolar	VAL 182 - VAL 257	TA01 - TB01	82.925
Nonpolar	LYS 394 - PRO 348	TA01 - TB01	82.002
Nonpolar	GTP 1 - ASN 228	GTP - TA00	100.000
Nonpolar	GTP 1 - THR 145	GTP - TA00	100.000
Nonpolar	GTP 1 - ALA 12	GTP - TA00	100.000

Table 4.4: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GTP 1 - GLN 11	GTP - TA00	100.000
Nonpolar	GTP 1 - GLY 143	GTP - TA00	99.997
Nonpolar	GTP 1 - GLY 146	GTP - TA00	99.995
Nonpolar	GTP 1 - ASP 69	GTP - TA00	99.847
Nonpolar	GTP 1 - GLY 144	GTP - TA00	99.485
Nonpolar	GTP 1 - ASN 206	GTP - TA00	99.127
Nonpolar	GTP 1 - TYR 224	GTP - TA00	98.712
Nonpolar	GTP 1 - SER 140	GTP - TA00	97.272
Nonpolar	GTP 1 - THR 179	GTP - TA00	96.097
Nonpolar	GTP 1 - GLY 10	GTP - TA00	93.570
Nonpolar	GTP 1 - ASN 101	GTP - TA00	91.252
Nonpolar	GTP 1 - GLN 15	GTP - TA00	89.887
Nonpolar	GTP 1 - VAL 177	GTP - TA00	85.430
Nonpolar	GTP 1 - ALA 100	GTP - TA00	81.075
Nonpolar	GDP 1 - ASN 228	GDP - TB00	99.987
Nonpolar	GDP 1 - TYR 224	GDP - TB00	98.117
Nonpolar	GDP 1 - CYS 12	GDP - TB00	92.292
Nonpolar	GDP 1 - GLY 143	GDP - TB00	91.475
Nonpolar	GTP 2 - ASN 228	GTP - TA01	100.000
Nonpolar	GTP 2 - GLY 146	GTP - TA01	100.000
Nonpolar	GTP 2 - THR 145	GTP - TA01	100.000
Nonpolar	GTP 2 - GLY 144	GTP - TA01	100.000
Nonpolar	GTP 2 - GLY 143	GTP - TA01	100.000

Table 4.4: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GTP 2 - ALA 12	GTP - TA01	100.000
Nonpolar	GTP 2 - GLN 11	GTP - TA01	100.000
Nonpolar	GTP 2 - ASN 101	GTP - TA01	99.997
Nonpolar	GTP 2 - ASP 69	GTP - TA01	99.827
Nonpolar	GTP 2 - SER 140	GTP - TA01	99.325
Nonpolar	GTP 2 - THR 179	GTP - TA01	99.175
Nonpolar	GTP 2 - GLU 183	GTP - TA01	99.000
Nonpolar	GTP 2 - ASN 206	GTP - TA01	96.132
Nonpolar	GTP 2 - TYR 224	GTP - TA01	95.777
Nonpolar	GTP 2 - GLY 10	GTP - TA01	95.332
Nonpolar	GTP 2 - VAL 177	GTP - TA01	81.942
Nonpolar	GDP 2 - ASN 228	GDP - TB01	100.000
Nonpolar	GDP 2 - ASN 206	GDP - TB01	99.937
Nonpolar	GDP 2 - TYR 224	GDP - TB01	99.180
Nonpolar	GDP 2 - SER 140	GDP - TB01	98.515
Nonpolar	GDP 2 - CYS 12	GDP - TB01	95.817
Nonpolar	GDP 2 - GLY 143	GDP - TB01	95.157
Nonpolar	GDP 2 - GLU 183	GDP - TB01	91.235
End of Table 4.4			

Table 4.5: Contacts Present in 3RYF 4-Dimer Microtubule Protofilament.

Contacts Present in 3RYF 4-Dimer System			
Contact Type	Contact	Domain	% Occupancy
Polar	PHE 404 - PRO 261	TA00 - TB00	99.143
Polar	ARG 221 - ASP 329	TA00 - TB00	99.005
Polar	GLU 71 - LYS 254	TA00 - TB00	89.580
Polar	ASP 98 - ARG 253	TA00 - TB00	88.390
Polar	VAL 181 - ASN 258	TA00 - TB00	87.152
Polar	PHE 404 - PRO 261	TB00 - TA01	99.119
Polar	THR 180 - ASN 258	TB00 - TA01	95.728
Polar	ASN 101 - ASN 258	TB00 - TA01	89.214
Polar	ARG 401 - TYR 262	TB00 - TA01	89.104
Polar	GLU 411 - LYS 163	TB00 - TA01	86.104
Polar	GLY 100 - THR 257	TB00 - TA01	81.928
Polar	PHE 404 - PRO 261	TA01 - TB01	98.586
Polar	ARG 221 - ASP 329	TA01 - TB01	96.862
Polar	GLU 71 - LYS 254	TA01 - TB01	94.038
Polar	ASP 98 - ARG 253	TA01 - TB01	90.619
Polar	VAL 181 - ASN 258	TA01 - TB01	84.114
Polar	PHE 404 - PRO 261	TB01 - TA02	99.067
Polar	ASN 101 - ASN 258	TB01 - TA02	89.171
Polar	THR 180 - ASN 258	TB01 - TA02	84.756
Polar	GLY 100 - THR 257	TB01 - TA02	82.375
Polar	VAL 181 - ASN 258	TA02 - TB02	98.176
Polar	PHE 404 - PRO 261	TA02 - TB02	96.086

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Polar	ARG 221 - ASP 329	TA02 - TB02	92.590
Polar	PHE 404 - PRO 261	TB02 - TA03	98.257
Polar	GLU 71 - ARG 2	TB02 - TA03	91.990
Polar	PHE 404 - PRO 261	TA03 - TB03	99.086
Polar	ARG 221 - ASP 329	TA03 - TB03	98.062
Polar	GLU 97 - ARG 164	TA03 - TB03	92.390
Polar	GLU 71 - LYS 254	TA03 - TB03	91.719
Polar	VAL 181 - ASN 258	TA03 - TB03	89.204
Polar	ASP 98 - LYS 254	TA03 - TB03	88.438
Polar	GTP 1 - ASN 228	GTP - TA00	99.995
Polar	GTP 1 - THR 145	GTP - TA00	99.938
Polar	GTP 1 - ALA 12	GTP - TA00	99.848
Polar	GTP 1 - ASN 206	GTP - TA00	87.699
Polar	GTP 1 - GLN 11	GTP - TA00	82.775
Polar	GTP 2 - ASN 228	GTP - TB00	99.957
Polar	GTP 2 - CYS 12	GTP - TB00	94.414
Polar	GTP 3 - ASN 228	GTP - TA01	99.933
Polar	GTP 3 - THR 145	GTP - TA01	99.610
Polar	GTP 3 - ALA 12	GTP - TA01	99.514
Polar	GTP 3 - ASN 206	GTP - TA01	94.481
Polar	GTP 4 - ASN 228	GTP - TB01	98.057
Polar	GTP 4 - CYS 12	GTP - TB01	91.852
Polar	GTP 5 - ASN 228	GTP - TA02	99.971

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Polar	GTP 5 - ALA 12	GTP - TA02	99.390
Polar	GTP 5 - ASN 206	GTP - TA02	92.528
Polar	GTP 6 - THR 145	GTP - TB02	100.000
Polar	GTP 6 - ASN 228	GTP - TB02	99.905
Polar	GTP 6 - GLN 11	GTP - TB02	99.762
Polar	GTP 6 - SER 140	GTP - TB02	98.262
Polar	GTP 6 - GLY 146	GTP - TB02	98.176
Polar	GTP 6 - ASN 206	GTP - TB02	97.128
Polar	GTP 6 - CYS 12	GTP - TB02	96.624
Polar	GTP 6 - GLU 183	GTP - TB02	95.714
Polar	GTP 6 - GLY 144	GTP - TB02	93.933
Polar	GTP 7 - ASN 228	GTP - TA03	99.971
Polar	GTP 7 - GLY 146	GTP - TA03	99.395
Polar	GTP 7 - ASN 206	GTP - TA03	94.795
Polar	GTP 7 - ALA 12	GTP - TA03	94.662
Polar	GTP 7 - GLN 11	GTP - TA03	94.190
Polar	GTP 7 - THR 145	GTP - TA03	93.695
Polar	GTP 7 - GLY 144	GTP - TA03	91.538
Polar	GTP 8 - ASN 228	GTP - TB03	99.767
Polar	GTP 8 - ASN 101	GTP - TB03	98.881
Polar	GTP 8 - CYS 12	GTP - TB03	96.362
Polar	GTP 8 - GLY 144	GTP - TB03	94.038
Polar	GTP 8 - GLY 146	GTP - TB03	82.847

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	PHE 404 - PRO 261	TA00 - TB00	100.000
Nonpolar	TRP 407 - VAL 260	TA00 - TB00	99.905
Nonpolar	PHE 404 - ILE 347	TA00 - TB00	99.762
Nonpolar	ARG 221 - ASP 329	TA00 - TB00	99.214
Nonpolar	VAL 181 - ASN 258	TA00 - TB00	98.671
Nonpolar	MET 398 - PRO 348	TA00 - TB00	98.605
Nonpolar	LEU 397 - TRP 346	TA00 - TB00	98.381
Nonpolar	ALA 180 - ASN 258	TA00 - TB00	98.138
Nonpolar	LYS 401 - PHE 262	TA00 - TB00	97.252
Nonpolar	THR 179 - LEU 248	TA00 - TB00	96.243
Nonpolar	ARG 221 - MET 325	TA00 - TB00	95.738
Nonpolar	HIS 406 - PRO 263	TA00 - TB00	95.576
Nonpolar	PRO 175 - ASN 349	TA00 - TB00	95.462
Nonpolar	LYS 394 - PRO 348	TA00 - TB00	94.995
Nonpolar	ASN 101 - LYS 254	TA00 - TB00	94.324
Nonpolar	LEU 397 - PRO 348	TA00 - TB00	93.785
Nonpolar	ALA 100 - ARG 253	TA00 - TB00	93.695
Nonpolar	SER 178 - LYS 352	TA00 - TB00	93.485
Nonpolar	LYS 401 - ALA 438	TA00 - TB00	92.790
Nonpolar	GLU 220 - LYS 326	TA00 - TB00	92.581
Nonpolar	ARG 221 - LYS 326	TA00 - TB00	91.419
Nonpolar	HIS 406 - VAL 260	TA00 - TB00	91.085
Nonpolar	PHE 404 - VAL 257	TA00 - TB00	90.676

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GLU 71 - LYS 254	TA00 - TB00	90.452
Nonpolar	TRP 407 - VAL 257	TA00 - TB00	89.828
Nonpolar	ASP 98 - ARG 253	TA00 - TB00	89.442
Nonpolar	VAL 182 - VAL 257	TA00 - TB00	89.242
Nonpolar	ALA 100 - LYS 254	TA00 - TB00	89.085
Nonpolar	TRP 407 - ALA 256	TA00 - TB00	89.014
Nonpolar	THR 179 - LYS 352	TA00 - TB00	80.885
Nonpolar	VAL 181 - LYS 352	TA00 - TB00	80.651
Nonpolar	MET 398 - ILE 347	TA00 - TB00	80.556
Nonpolar	PHE 404 - PRO 261	TB00 - TA01	100.000
Nonpolar	THR 180 - ASN 258	TB00 - TA01	99.910
Nonpolar	TRP 407 - VAL 260	TB00 - TA01	99.729
Nonpolar	ASP 179 - LYS 352	TB00 - TA01	99.624
Nonpolar	ASN 101 - ASN 258	TB00 - TA01	99.476
Nonpolar	ARG 401 - TYR 262	TB00 - TA01	99.405
Nonpolar	GLY 100 - GLU 254	TB00 - TA01	98.319
Nonpolar	VAL 181 - PRO 348	TB00 - TA01	98.128
Nonpolar	ASN 101 - LYS 352	TB00 - TA01	97.724
Nonpolar	TRP 407 - GLN 256	TB00 - TA01	97.271
Nonpolar	GLY 100 - THR 257	TB00 - TA01	96.971
Nonpolar	SER 178 - GLY 350	TB00 - TA01	96.143
Nonpolar	GLY 100 - THR 253	TB00 - TA01	94.714
Nonpolar	ALA 397 - TRP 346	TB00 - TA01	93.204

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	ASN 101 - GLU 254	TB00 - TA01	92.295
Nonpolar	ALA 403 - TRP 346	TB00 - TA01	92.276
Nonpolar	ASP 179 - PHE 351	TB00 - TA01	91.390
Nonpolar	MET 398 - PRO 348	TB00 - TA01	90.447
Nonpolar	VAL 182 - THR 257	TB00 - TA01	90.190
Nonpolar	HIS 406 - PRO 263	TB00 - TA01	89.685
Nonpolar	GLN 394 - PRO 348	TB00 - TA01	89.371
Nonpolar	VAL 181 - ALA 314	TB00 - TA01	88.257
Nonpolar	GLU 411 - LYS 163	TB00 - TA01	87.133
Nonpolar	PRO 184 - PRO 348	TB00 - TA01	86.757
Nonpolar	THR 221 - LYS 326	TB00 - TA01	84.890
Nonpolar	ARG 401 - GLU 434	TB00 - TA01	84.709
Nonpolar	LYS 402 - TYR 262	TB00 - TA01	82.099
Nonpolar	PHE 404 - ASN 258	TB00 - TA01	81.971
Nonpolar	TRP 407 - ASP 199	TB00 - TA01	80.709
Nonpolar	PHE 404 - PRO 261	TA01 - TB01	100.000
Nonpolar	TRP 407 - VAL 260	TA01 - TB01	99.919
Nonpolar	PHE 404 - ILE 347	TA01 - TB01	99.700
Nonpolar	LYS 394 - PRO 348	TA01 - TB01	99.700
Nonpolar	LEU 397 - TRP 346	TA01 - TB01	98.938
Nonpolar	ALA 180 - ASN 258	TA01 - TB01	98.762
Nonpolar	LYS 401 - PHE 262	TA01 - TB01	98.467
Nonpolar	VAL 181 - ASN 258	TA01 - TB01	98.100

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	MET 398 - PRO 348	TA01 - TB01	97.605
Nonpolar	MET 398 - ILE 347	TA01 - TB01	97.590
Nonpolar	ARG 221 - ASP 329	TA01 - TB01	97.052
Nonpolar	VAL 182 - VAL 257	TA01 - TB01	95.419
Nonpolar	TRP 407 - ALA 256	TA01 - TB01	95.019
Nonpolar	GLU 71 - LYS 254	TA01 - TB01	94.681
Nonpolar	LYS 401 - THR 439	TA01 - TB01	93.814
Nonpolar	HIS 406 - PRO 263	TA01 - TB01	92.333
Nonpolar	LYS 401 - ALA 438	TA01 - TB01	91.728
Nonpolar	ARG 221 - LYS 326	TA01 - TB01	91.557
Nonpolar	TRP 407 - VAL 257	TA01 - TB01	91.428
Nonpolar	ASP 98 - ARG 253	TA01 - TB01	90.871
Nonpolar	ALA 100 - ARG 253	TA01 - TB01	90.800
Nonpolar	GLU 220 - LYS 326	TA01 - TB01	90.366
Nonpolar	PHE 404 - VAL 257	TA01 - TB01	89.209
Nonpolar	THR 179 - LEU 248	TA01 - TB01	88.823
Nonpolar	ALA 100 - LYS 254	TA01 - TB01	88.771
Nonpolar	SER 178 - LYS 352	TA01 - TB01	88.761
Nonpolar	PRO 175 - ASN 349	TA01 - TB01	87.942
Nonpolar	ASN 101 - LYS 254	TA01 - TB01	86.857
Nonpolar	LEU 397 - ALA 440	TA01 - TB01	83.571
Nonpolar	ALA 403 - TRP 346	TA01 - TB01	81.675
Nonpolar	ARG 402 - PHE 262	TA01 - TB01	80.342

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	PHE 404 - PRO 261	TB01 - TA02	100.000
Nonpolar	TRP 407 - VAL 260	TB01 - TA02	99.952
Nonpolar	ARG 401 - TYR 262	TB01 - TA02	99.652
Nonpolar	THR 180 - ASN 258	TB01 - TA02	99.167
Nonpolar	ASP 179 - LYS 352	TB01 - TA02	99.014
Nonpolar	ASN 101 - ASN 258	TB01 - TA02	98.048
Nonpolar	TRP 407 - GLN 256	TB01 - TA02	97.490
Nonpolar	GLY 100 - GLU 254	TB01 - TA02	95.795
Nonpolar	ASN 101 - LYS 352	TB01 - TA02	95.147
Nonpolar	VAL 181 - PRO 348	TB01 - TA02	94.324
Nonpolar	ALA 397 - TRP 346	TB01 - TA02	94.295
Nonpolar	GLY 100 - THR 257	TB01 - TA02	93.752
Nonpolar	SER 178 - GLY 350	TB01 - TA02	91.676
Nonpolar	VAL 181 - ASN 258	TB01 - TA02	90.342
Nonpolar	MET 398 - PRO 348	TB01 - TA02	90.138
Nonpolar	ASN 101 - GLU 254	TB01 - TA02	89.085
Nonpolar	ALA 403 - TRP 346	TB01 - TA02	88.919
Nonpolar	HIS 406 - PRO 263	TB01 - TA02	88.509
Nonpolar	ARG 401 - TRP 346	TB01 - TA02	88.285
Nonpolar	PHE 404 - THR 257	TB01 - TA02	88.028
Nonpolar	VAL 182 - THR 257	TB01 - TA02	87.004
Nonpolar	MET 398 - TRP 346	TB01 - TA02	82.890
Nonpolar	GLY 100 - THR 253	TB01 - TA02	81.990

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	ASN 101 - THR 257	TB01 - TA02	81.975
Nonpolar	TRP 407 - THR 257	TB01 - TA02	81.523
Nonpolar	PRO 184 - PRO 348	TB01 - TA02	81.442
Nonpolar	PHE 404 - PRO 261	TA02 - TB02	100.000
Nonpolar	VAL 181 - ASN 258	TA02 - TB02	99.952
Nonpolar	TRP 407 - VAL 260	TA02 - TB02	99.724
Nonpolar	LYS 394 - PRO 348	TA02 - TB02	99.290
Nonpolar	ALA 100 - LYS 254	TA02 - TB02	98.200
Nonpolar	PHE 404 - ILE 347	TA02 - TB02	97.824
Nonpolar	LEU 397 - TRP 346	TA02 - TB02	97.800
Nonpolar	LYS 401 - PHE 262	TA02 - TB02	97.405
Nonpolar	SER 178 - LYS 352	TA02 - TB02	97.362
Nonpolar	ALA 180 - ASN 258	TA02 - TB02	97.119
Nonpolar	VAL 182 - ASN 258	TA02 - TB02	97.100
Nonpolar	ASN 101 - ASN 258	TA02 - TB02	96.324
Nonpolar	THR 179 - LYS 352	TA02 - TB02	96.000
Nonpolar	MET 398 - PRO 348	TA02 - TB02	95.557
Nonpolar	THR 179 - LEU 248	TA02 - TB02	94.938
Nonpolar	ARG 221 - ASP 329	TA02 - TB02	94.519
Nonpolar	TRP 407 - VAL 257	TA02 - TB02	94.505
Nonpolar	PRO 175 - LYS 352	TA02 - TB02	94.166
Nonpolar	PHE 404 - VAL 257	TA02 - TB02	93.914
Nonpolar	HIS 406 - PRO 263	TA02 - TB02	93.752

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	ALA 100 - ARG 253	TA02 - TB02	92.695
Nonpolar	ARG 221 - LYS 326	TA02 - TB02	92.481
Nonpolar	ALA 403 - PRO 261	TA02 - TB02	91.733
Nonpolar	ASN 101 - LYS 254	TA02 - TB02	91.357
Nonpolar	LEU 397 - PRO 348	TA02 - TB02	89.657
Nonpolar	PRO 175 - ASN 349	TA02 - TB02	89.438
Nonpolar	ARG 221 - MET 325	TA02 - TB02	88.509
Nonpolar	GLU 97 - ARG 253	TA02 - TB02	83.699
Nonpolar	PHE 404 - ASN 258	TA02 - TB02	82.123
Nonpolar	VAL 182 - VAL 257	TA02 - TB02	81.580
Nonpolar	PHE 404 - PRO 261	TB02 - TA03	100.000
Nonpolar	TRP 407 - VAL 260	TB02 - TA03	99.638
Nonpolar	ARG 401 - TYR 262	TB02 - TA03	99.590
Nonpolar	ASP 179 - LYS 352	TB02 - TA03	99.090
Nonpolar	TRP 407 - GLN 256	TB02 - TA03	97.852
Nonpolar	THR 180 - ASN 258	TB02 - TA03	96.033
Nonpolar	GLY 100 - GLU 254	TB02 - TA03	94.647
Nonpolar	ALA 397 - TRP 346	TB02 - TA03	94.471
Nonpolar	GLU 71 - ARG 2	TB02 - TA03	92.147
Nonpolar	MET 398 - TRP 346	TB02 - TA03	91.919
Nonpolar	GLN 394 - PRO 348	TB02 - TA03	90.000
Nonpolar	PRO 175 - THR 349	TB02 - TA03	89.804
Nonpolar	HIS 406 - PRO 263	TB02 - TA03	89.609

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	VAL 181 - PRO 348	TB02 - TA03	87.890
Nonpolar	TRP 407 - THR 257	TB02 - TA03	87.085
Nonpolar	GLY 100 - THR 257	TB02 - TA03	86.966
Nonpolar	ARG 401 - TRP 346	TB02 - TA03	86.347
Nonpolar	GLY 100 - THR 253	TB02 - TA03	83.747
Nonpolar	VAL 182 - THR 257	TB02 - TA03	81.471
Nonpolar	PRO 184 - PRO 348	TB02 - TA03	81.456
Nonpolar	ALA 403 - PRO 261	TB02 - TA03	81.437
Nonpolar	MET 398 - PRO 348	TB02 - TA03	81.413
Nonpolar	PHE 404 - PRO 261	TA03 - TB03	100.000
Nonpolar	PHE 404 - ILE 347	TA03 - TB03	99.881
Nonpolar	TRP 407 - VAL 260	TA03 - TB03	99.700
Nonpolar	ARG 221 - ASP 329	TA03 - TB03	99.600
Nonpolar	VAL 181 - ASN 258	TA03 - TB03	99.595
Nonpolar	MET 398 - PRO 348	TA03 - TB03	99.271
Nonpolar	LYS 401 - PHE 262	TA03 - TB03	98.848
Nonpolar	GLU 71 - LYS 254	TA03 - TB03	98.105
Nonpolar	LEU 397 - PRO 348	TA03 - TB03	97.786
Nonpolar	THR 179 - LEU 248	TA03 - TB03	97.457
Nonpolar	VAL 182 - VAL 257	TA03 - TB03	96.852
Nonpolar	SER 178 - LYS 352	TA03 - TB03	96.471
Nonpolar	ALA 100 - LYS 254	TA03 - TB03	96.205
Nonpolar	ARG 221 - MET 325	TA03 - TB03	94.709

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	ALA 100 - ARG 253	TA03 - TB03	94.690
Nonpolar	ASP 98 - LYS 254	TA03 - TB03	94.690
Nonpolar	LYS 394 - PRO 348	TA03 - TB03	93.166
Nonpolar	GLU 97 - ARG 164	TA03 - TB03	92.990
Nonpolar	ARG 221 - LYS 326	TA03 - TB03	91.833
Nonpolar	VAL 181 - LYS 352	TA03 - TB03	91.809
Nonpolar	GLU 220 - LYS 326	TA03 - TB03	91.752
Nonpolar	LEU 397 - TRP 346	TA03 - TB03	90.433
Nonpolar	PHE 404 - VAL 257	TA03 - TB03	88.557
Nonpolar	HIS 406 - PRO 263	TA03 - TB03	87.814
Nonpolar	ALA 180 - ASN 258	TA03 - TB03	87.461
Nonpolar	LYS 401 - TRP 346	TA03 - TB03	87.171
Nonpolar	TRP 407 - ALA 256	TA03 - TB03	86.966
Nonpolar	ALA 403 - PRO 261	TA03 - TB03	86.223
Nonpolar	ALA 403 - ILE 347	TA03 - TB03	86.209
Nonpolar	TRP 407 - VAL 257	TA03 - TB03	85.633
Nonpolar	THR 179 - LYS 352	TA03 - TB03	84.347
Nonpolar	PRO 175 - ASN 349	TA03 - TB03	82.633
Nonpolar	THR 179 - GLN 247	TA03 - TB03	82.609
Nonpolar	PHE 404 - VAL 260	TA03 - TB03	82.085
Nonpolar	PRO 175 - LYS 352	TA03 - TB03	81.618
Nonpolar	GLU 97 - MET 1	TA03 - TB03	81.204
Nonpolar	GTP 1 - ASN 228	GTP - TA00	100.000

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GTP 1 - GLY 146	GTP - TA00	100.000
Nonpolar	GTP 1 - THR 145	GTP - TA00	100.000
Nonpolar	GTP 1 - ALA 12	GTP - TA00	100.000
Nonpolar	GTP 1 - GLN 11	GTP - TA00	100.000
Nonpolar	GTP 1 - GLY 143	GTP - TA00	99.995
Nonpolar	GTP 1 - ASN 101	GTP - TA00	99.995
Nonpolar	GTP 1 - GLY 144	GTP - TA00	99.981
Nonpolar	GTP 1 - ASP 69	GTP - TA00	99.952
Nonpolar	GTP 1 - SER 178	GTP - TA00	99.757
Nonpolar	GTP 1 - GLU 183	GTP - TA00	99.619
Nonpolar	GTP 1 - TYR 224	GTP - TA00	97.800
Nonpolar	GTP 1 - SER 140	GTP - TA00	96.867
Nonpolar	GTP 1 - ASN 206	GTP - TA00	95.576
Nonpolar	GTP 1 - GLY 10	GTP - TA00	90.004
Nonpolar	GTP 1 - GLN 15	GTP - TA00	87.342
Nonpolar	GTP 2 - THR 145	GTP - TB00	100.000
Nonpolar	GTP 2 - ASP 69	GTP - TB00	100.000
Nonpolar	GTP 2 - CYS 12	GTP - TB00	100.000
Nonpolar	GTP 2 - GLN 11	GTP - TB00	100.000
Nonpolar	GTP 2 - ASN 228	GTP - TB00	99.995
Nonpolar	GTP 2 - GLY 143	GTP - TB00	99.990
Nonpolar	GTP 2 - GLY 146	GTP - TB00	99.952
Nonpolar	GTP 2 - GLY 144	GTP - TB00	99.757

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GTP 2 - ASP 179	GTP - TB00	99.448
Nonpolar	GTP 2 - TYR 224	GTP - TB00	97.305
Nonpolar	GTP 2 - ALA 99	GTP - TB00	95.052
Nonpolar	GTP 2 - GLY 10	GTP - TB00	86.347
Nonpolar	GTP 3 - ASN 0228	GTP - TA01	100.000
Nonpolar	GTP 3 - GLY 0146	GTP - TA01	100.000
Nonpolar	GTP 3 - THR 0145	GTP - TA01	100.000
Nonpolar	GTP 3 - ALA 0012	GTP - TA01	100.000
Nonpolar	GTP 3 - GLN 0011	GTP - TA01	100.000
Nonpolar	GTP 3 - GLY 0144	GTP - TA01	99.990
Nonpolar	GTP 3 - GLY 0143	GTP - TA01	99.971
Nonpolar	GTP 3 - ASP 0069	GTP - TA01	99.881
Nonpolar	GTP 3 - ASN 0101	GTP - TA01	99.467
Nonpolar	GTP 3 - ASN 0206	GTP - TA01	99.057
Nonpolar	GTP 3 - TYR 0224	GTP - TA01	98.690
Nonpolar	GTP 3 - SER 0178	GTP - TA01	92.547
Nonpolar	GTP 3 - SER 0140	GTP - TA01	91.942
Nonpolar	GTP 3 - GLN 0015	GTP - TA01	89.985
Nonpolar	GTP 3 - ALA 0099	GTP - TA01	89.133
Nonpolar	GTP 3 - GLU 0183	GTP - TA01	89.114
Nonpolar	GTP 3 - VAL 0177	GTP - TA01	83.775
Nonpolar	GTP 4 - THR 0145	GTP - TB01	100.000
Nonpolar	GTP 4 - GLN 0011	GTP - TB01	100.000

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GTP 4 - CYS 0012	GTP - TB01	99.995
Nonpolar	GTP 4 - ASP 0069	GTP - TB01	99.986
Nonpolar	GTP 4 - GLY 0144	GTP - TB01	99.748
Nonpolar	GTP 4 - GLY 0143	GTP - TB01	99.519
Nonpolar	GTP 4 - GLY 0146	GTP - TB01	99.490
Nonpolar	GTP 4 - GLY 0010	GTP - TB01	98.829
Nonpolar	GTP 4 - ASN 0228	GTP - TB01	98.819
Nonpolar	GTP 4 - SER 0140	GTP - TB01	97.724
Nonpolar	GTP 4 - TYR 0224	GTP - TB01	96.643
Nonpolar	GTP 4 - ASP 0179	GTP - TB01	93.357
Nonpolar	GTP 5 - ASN 0228	GTP - TA02	100.000
Nonpolar	GTP 5 - THR 0145	GTP - TA02	100.000
Nonpolar	GTP 5 - GLY 0143	GTP - TA02	100.000
Nonpolar	GTP 5 - ALA 0012	GTP - TA02	100.000
Nonpolar	GTP 5 - GLN 0011	GTP - TA02	100.000
Nonpolar	GTP 5 - GLY 0146	GTP - TA02	99.986
Nonpolar	GTP 5 - ASP 0069	GTP - TA02	99.871
Nonpolar	GTP 5 - GLY 0010	GTP - TA02	99.462
Nonpolar	GTP 5 - ASN 0206	GTP - TA02	99.276
Nonpolar	GTP 5 - GLY 0144	GTP - TA02	98.809
Nonpolar	GTP 5 - SER 0140	GTP - TA02	98.009
Nonpolar	GTP 5 - TYR 0224	GTP - TA02	95.990
Nonpolar	GTP 5 - GLU 0183	GTP - TA02	92.095

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GTP 5 - GLN 0015	GTP - TA02	88.142
Nonpolar	GTP 5 - ALA 0099	GTP - TA02	86.647
Nonpolar	GTP 5 - ASN 0101	GTP - TA02	83.290
Nonpolar	GTP 5 - SER 0178	GTP - TA02	80.694
Nonpolar	GTP 6 - ASN 0228	GTP - TB02	100.000
Nonpolar	GTP 6 - THR 0145	GTP - TB02	100.000
Nonpolar	GTP 6 - GLY 0143	GTP - TB02	100.000
Nonpolar	GTP 6 - ASP 0069	GTP - TB02	100.000
Nonpolar	GTP 6 - CYS 0012	GTP - TB02	100.000
Nonpolar	GTP 6 - GLN 0011	GTP - TB02	100.000
Nonpolar	GTP 6 - SER 0140	GTP - TB02	99.995
Nonpolar	GTP 6 - GLU 0183	GTP - TB02	99.971
Nonpolar	GTP 6 - GLY 0146	GTP - TB02	99.957
Nonpolar	GTP 6 - GLY 0144	GTP - TB02	99.957
Nonpolar	GTP 6 - ASN 0206	GTP - TB02	99.924
Nonpolar	GTP 6 - ALA 0099	GTP - TB02	99.395
Nonpolar	GTP 6 - GLY 0010	GTP - TB02	97.690
Nonpolar	GTP 6 - TYR 0224	GTP - TB02	95.852
Nonpolar	GTP 6 - GLY 0142	GTP - TB02	94.433
Nonpolar	GTP 6 - SER 0178	GTP - TB02	80.347
Nonpolar	GTP 7 - ASN 0228	GTP - TA03	100.000
Nonpolar	GTP 7 - GLY 0146	GTP - TA03	100.000
Nonpolar	GTP 7 - THR 0145	GTP - TA03	100.000

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GTP 7 - GLY 0143	GTP - TA03	100.000
Nonpolar	GTP 7 - ALA 0012	GTP - TA03	100.000
Nonpolar	GTP 7 - GLN 0011	GTP - TA03	99.995
Nonpolar	GTP 7 - ASP 0069	GTP - TA03	99.962
Nonpolar	GTP 7 - GLY 0144	GTP - TA03	99.695
Nonpolar	GTP 7 - ASN 0206	GTP - TA03	98.995
Nonpolar	GTP 7 - GLY 0010	GTP - TA03	98.943
Nonpolar	GTP 7 - SER 0178	GTP - TA03	97.705
Nonpolar	GTP 7 - TYR 0224	GTP - TA03	97.567
Nonpolar	GTP 7 - ASN 0101	GTP - TA03	94.885
Nonpolar	GTP 7 - PRO 0173	GTP - TA03	87.276
Nonpolar	GTP 7 - SER 0140	GTP - TA03	85.876
Nonpolar	GTP 7 - ILE 0171	GTP - TA03	83.694
Nonpolar	GTP 8 - THR 0145	GTP - TB03	100.000
Nonpolar	GTP 8 - GLU 0071	GTP - TB03	100.000
Nonpolar	GTP 8 - GLY 0143	GTP - TB03	99.995
Nonpolar	GTP 8 - ASN 0228	GTP - TB03	99.986
Nonpolar	GTP 8 - GLY 0144	GTP - TB03	99.910
Nonpolar	GTP 8 - GLN 0011	GTP - TB03	99.814
Nonpolar	GTP 8 - ASN 0101	GTP - TB03	99.771
Nonpolar	GTP 8 - CYS 0012	GTP - TB03	99.724
Nonpolar	GTP 8 - GLY 0146	GTP - TB03	99.576
Nonpolar	GTP 8 - TYR 0224	GTP - TB03	96.728

Table 4.5: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GTP 8 - ALA 0099	GTP - TB03	95.066
Nonpolar	GTP 8 - GLN 0015	GTP - TB03	87.861
End of Table 4.5			

Table 4.6: Contacts Present in 3RYI 4-Dimer Microtubule Protofilament.

Contacts Present in 3RYI 4-Dimer System			
Contact Type	Contact	Domain	% Occupancy
Polar	ASP 98 - MET 1	TA00 - TB00	99.752
Polar	PHE 404 - PRO 261	TA00 - TB00	99.567
Polar	ARG 221 - ASP 329	TA00 - TB00	98.357
Polar	ARG 105 - ASP 163	TA00 - TB00	97.762
Polar	GLU 71 - MET 1	TA00 - TB00	96.128
Polar	THR 179 - ASN 258	TA00 - TB00	95.319
Polar	ASN 101 - LYS 254	TA00 - TB00	93.614
Polar	GLU 71 - ARG 2	TA00 - TB00	93.366
Polar	SER 178 - LYS 352	TA00 - TB00	84.337
Polar	ASP 76 - ARG 2	TA00 - TB00	80.694
Polar	GLU 71 - ARG 2	TB00 - TA01	99.286
Polar	PHE 404 - PRO 261	TB00 - TA01	97.333
Polar	THR 180 - ASN 258	TB00 - TA01	82.923
Polar	PHE 404 - PRO 261	TA01 - TB01	99.286
Polar	VAL 181 - ASN 258	TA01 - TB01	98.543
Polar	GLU 97 - ARG 253	TA01 - TB01	83.871

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Polar	ASN 101 - ASN 258	TA01 - TB01	80.218
Polar	PHE 404 - PRO 261	TB01 - TA02	99.048
Polar	ASP 179 - LYS 352	TB01 - TA02	93.157
Polar	THR 180 - ASN 258	TB01 - TA02	84.275
Polar	ARG 214 - ASP 329	TA02 - TB02	99.857
Polar	PHE 404 - PRO 261	TA02 - TB02	98.938
Polar	ARG 215 - GLU 330	TA02 - TB02	89.538
Polar	ASP 98 - ARG 253	TA02 - TB02	88.499
Polar	GLU 97 - ARG 253	TA02 - TB02	83.071
Polar	GLU 71 - ARG 2	TB02 - TA03	99.148
Polar	PHE 404 - PRO 261	TB02 - TA03	99.019
Polar	ASN 101 - ASN 258	TB02 - TA03	95.081
Polar	ARG 401 - VAL 440	TB02 - TA03	83.542
Polar	GLY 100 - THR 257	TB02 - TA03	81.799
Polar	ASP 98 - LYS 254	TA03 - TB03	99.810
Polar	PHE 404 - PRO 261	TA03 - TB03	98.248
Polar	GLU 71 - LYS 254	TA03 - TB03	97.762
Polar	ARG 221 - ASP 329	TA03 - TB03	96.657
Polar	VAL 181 - ASN 258	TA03 - TB03	88.009
Polar	TRP 407 - VAL 260	TA03 - TB03	82.090
Polar	GTP 1 - ASN 228	GTP - TA00	99.829
Polar	GTP 1 - ALA 12	GTP - TA00	99.795
Polar	GTP 1 - GLN 11	GTP - TA00	90.252

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Polar	GDP 1 - ASN 228	GDP - TB00	96.028
Polar	GTP 2 - ASN 228	GTP - TA01	99.862
Polar	GTP 2 - ALA 12	GTP - TA01	95.395
Polar	GDP 2 - ASN 228	GDP - TB01	99.986
Polar	GDP 2 - ASN 206	GDP - TB01	88.442
Polar	GTP 3 - ALA 12	GTP - TA02	99.181
Polar	GTP 3 - ASN 228	GTP - TA02	96.514
Polar	GDP 3 - ASN 228	GDP - TB02	99.981
Polar	GDP 3 - ASN 206	GDP - TB02	97.843
Polar	GTP 4 - GLY 144	GTP - TA03	99.995
Polar	GTP 4 - ASN 101	GTP - TA03	99.986
Polar	GTP 4 - ALA 12	GTP - TA03	99.895
Polar	GTP 4 - GLN 11	GTP - TA03	99.843
Polar	GTP 4 - ASN 228	GTP - TA03	99.643
Polar	GTP 4 - GLY 146	GTP - TA03	99.338
Polar	GTP 4 - ASN 206	GTP - TA03	83.766
Polar	GDP 4 - ASN 228	GDP - TB03	99.586
Polar	GDP 4 - GLY 144	GDP - TB03	98.671
Polar	GDP 4 - CYS 12	GDP - TB03	90.566
Polar	GDP 4 - ASN 206	GDP - TB03	87.095
Polar	GDP 4 - THR 145	GDP - TB03	86.152
Nonpolar	PHE 404 - PRO 261	TA00 - TB00	100.000
Nonpolar	ALA 100 - LYS 254	TA00 - TB00	100.000

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	ASP 98 - MET 1	TA00 - TB00	99.962
Nonpolar	GLU 71 - MET 1	TA00 - TB00	99.962
Nonpolar	TRP 407 - VAL 260	TA00 - TB00	99.948
Nonpolar	ALA 180 - ASN 258	TA00 - TB00	99.919
Nonpolar	THR 179 - ASN 258	TA00 - TB00	99.829
Nonpolar	ASN 101 - LYS 254	TA00 - TB00	99.767
Nonpolar	PHE 404 - ILE 347	TA00 - TB00	99.610
Nonpolar	THR 179 - LEU 248	TA00 - TB00	99.557
Nonpolar	GLU 97 - MET 1	TA00 - TB00	99.495
Nonpolar	ARG 221 - MET 325	TA00 - TB00	99.424
Nonpolar	LYS 394 - PRO 348	TA00 - TB00	98.752
Nonpolar	HIS 406 - VAL 260	TA00 - TB00	98.719
Nonpolar	ARG 105 - ASP 163	TA00 - TB00	98.600
Nonpolar	LYS 401 - PHE 262	TA00 - TB00	98.486
Nonpolar	ARG 221 - ASP 329	TA00 - TB00	98.386
Nonpolar	LEU 397 - TRP 346	TA00 - TB00	98.219
Nonpolar	SER 178 - LYS 352	TA00 - TB00	98.076
Nonpolar	ALA 100 - ARG 253	TA00 - TB00	97.786
Nonpolar	MET 398 - PRO 348	TA00 - TB00	97.700
Nonpolar	ASN 101 - VAL 257	TA00 - TB00	96.786
Nonpolar	TRP 407 - ALA 256	TA00 - TB00	95.843
Nonpolar	HIS 406 - PRO 263	TA00 - TB00	95.109
Nonpolar	THR 73 - ARG 2	TA00 - TB00	94.966

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	VAL 181 - ASN 258	TA00 - TB00	94.052
Nonpolar	GLU 71 - ARG 2	TA00 - TB00	94.047
Nonpolar	LEU 397 - PRO 348	TA00 - TB00	91.447
Nonpolar	ALA 180 - LYS 352	TA00 - TB00	90.514
Nonpolar	VAL 181 - LYS 352	TA00 - TB00	90.247
Nonpolar	VAL 181 - ILE 347	TA00 - TB00	89.961
Nonpolar	MET 398 - ILE 347	TA00 - TB00	89.499
Nonpolar	GLU 220 - LYS 326	TA00 - TB00	89.352
Nonpolar	LYS 401 - THR 439	TA00 - TB00	88.780
Nonpolar	PRO 72 - ARG 2	TA00 - TB00	88.204
Nonpolar	VAL 181 - ASN 350	TA00 - TB00	87.538
Nonpolar	ARG 221 - LYS 326	TA00 - TB00	85.452
Nonpolar	LYS 96 - CYS 131	TA00 - TB00	84.785
Nonpolar	LYS 401 - TRP 346	TA00 - TB00	84.404
Nonpolar	GLN 11 - GLN 247	TA00 - TB00	82.261
Nonpolar	ASP 76 - ARG 2	TA00 - TB00	81.151
Nonpolar	PHE 404 - VAL 257	TA00 - TB00	80.851
Nonpolar	TRP 407 - VAL 257	TA00 - TB00	80.761
Nonpolar	PHE 404 - PRO 261	TB00 - TA01	100.000
Nonpolar	TRP 407 - VAL 260	TB00 - TA01	99.924
Nonpolar	GLU 71 - ARG 2	TB00 - TA01	99.405
Nonpolar	THR 180 - ASN 258	TB00 - TA01	95.971
Nonpolar	ASN 101 - ASN 258	TB00 - TA01	94.700

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	ASN 101 - THR 257	TB00 - TA01	94.581
Nonpolar	TRP 407 - GLN 256	TB00 - TA01	94.019
Nonpolar	PRO 72 - ARG 2	TB00 - TA01	92.076
Nonpolar	GLY 100 - THR 257	TB00 - TA01	91.304
Nonpolar	ARG 401 - TYR 262	TB00 - TA01	90.719
Nonpolar	ASP 179 - LYS 352	TB00 - TA01	90.142
Nonpolar	ALA 397 - TRP 346	TB00 - TA01	89.057
Nonpolar	HIS 406 - PRO 263	TB00 - TA01	87.152
Nonpolar	MET 398 - TRP 346	TB00 - TA01	87.147
Nonpolar	GLY 100 - GLU 254	TB00 - TA01	86.923
Nonpolar	GLY 100 - THR 253	TB00 - TA01	85.790
Nonpolar	VAL 181 - GLY 350	TB00 - TA01	85.599
Nonpolar	ARG 401 - TRP 346	TB00 - TA01	83.494
Nonpolar	ASN 101 - GLU 254	TB00 - TA01	82.780
Nonpolar	PHE 404 - PRO 261	TA01 - TB01	100.000
Nonpolar	VAL 181 - ASN 258	TA01 - TB01	99.995
Nonpolar	PHE 404 - ILE 347	TA01 - TB01	99.581
Nonpolar	THR 179 - LEU 248	TA01 - TB01	99.533
Nonpolar	TRP 407 - VAL 260	TA01 - TB01	98.995
Nonpolar	LYS 401 - PHE 262	TA01 - TB01	98.995
Nonpolar	LYS 394 - PRO 348	TA01 - TB01	98.895
Nonpolar	LEU 397 - TRP 346	TA01 - TB01	98.524
Nonpolar	ALA 100 - LYS 254	TA01 - TB01	98.448

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	ALA 180 - ASN 258	TA01 - TB01	98.195
Nonpolar	MET 398 - PRO 348	TA01 - TB01	97.548
Nonpolar	ASN 101 - ASN 258	TA01 - TB01	97.324
Nonpolar	THR 179 - LYS 352	TA01 - TB01	97.219
Nonpolar	ASN 101 - LYS 254	TA01 - TB01	96.957
Nonpolar	SER 178 - LYS 352	TA01 - TB01	96.843
Nonpolar	TRP 407 - VAL 257	TA01 - TB01	96.186
Nonpolar	HIS 406 - PRO 263	TA01 - TB01	95.566
Nonpolar	PHE 404 - VAL 257	TA01 - TB01	95.500
Nonpolar	GLU 97 - ARG 253	TA01 - TB01	91.928
Nonpolar	LEU 397 - PRO 348	TA01 - TB01	90.271
Nonpolar	TRP 407 - ALA 256	TA01 - TB01	90.138
Nonpolar	MET 398 - ILE 347	TA01 - TB01	89.271
Nonpolar	ALA 100 - ARG 253	TA01 - TB01	89.204
Nonpolar	ASP 98 - ARG 253	TA01 - TB01	87.833
Nonpolar	VAL 182 - ASN 258	TA01 - TB01	87.580
Nonpolar	VAL 182 - VAL 257	TA01 - TB01	87.295
Nonpolar	ALA 100 - VAL 257	TA01 - TB01	85.204
Nonpolar	ARG 221 - LYS 326	TA01 - TB01	84.237
Nonpolar	ALA 403 - PRO 261	TA01 - TB01	82.875
Nonpolar	HIS 406 - VAL 260	TA01 - TB01	81.328
Nonpolar	PHE 404 - PRO 261	TB01 - TA02	100.000
Nonpolar	ASP 179 - LYS 352	TB01 - TA02	99.486

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	THR 180 - ASN 258	TB01 - TA02	99.362
Nonpolar	TRP 407 - GLN 256	TB01 - TA02	97.100
Nonpolar	VAL 181 - THR 349	TB01 - TA02	94.805
Nonpolar	ASN 101 - THR 257	TB01 - TA02	94.681
Nonpolar	TRP 407 - VAL 260	TB01 - TA02	94.528
Nonpolar	PRO 175 - THR 349	TB01 - TA02	93.490
Nonpolar	VAL 181 - ASN 258	TB01 - TA02	92.843
Nonpolar	ARG 401 - TYR 262	TB01 - TA02	92.319
Nonpolar	MET 398 - TRP 346	TB01 - TA02	91.438
Nonpolar	TRP 407 - THR 257	TB01 - TA02	90.490
Nonpolar	ALA 397 - TRP 346	TB01 - TA02	88.342
Nonpolar	ASN 101 - GLU 254	TB01 - TA02	87.833
Nonpolar	ALA 403 - TRP 346	TB01 - TA02	87.118
Nonpolar	GLY 100 - THR 253	TB01 - TA02	86.966
Nonpolar	HIS 406 - PRO 263	TB01 - TA02	86.090
Nonpolar	ALA 403 - TYR 262	TB01 - TA02	85.876
Nonpolar	SER 97 - ARG 2	TB01 - TA02	85.385
Nonpolar	ARG 401 - TRP 346	TB01 - TA02	84.542
Nonpolar	GLN 394 - PRO 348	TB01 - TA02	83.566
Nonpolar	TRP 407 - ASP 199	TB01 - TA02	82.009
Nonpolar	ALA 403 - PRO 261	TB01 - TA02	80.775
Nonpolar	ARG 401 - VAL 440	TB01 - TA02	80.513
Nonpolar	PHE 404 - PRO 261	TA02 - TB02	100.000

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	TRP 407 - VAL 260	TA02 - TB02	99.895
Nonpolar	ARG 214 - ASP 329	TA02 - TB02	99.886
Nonpolar	VAL 181 - ASN 258	TA02 - TB02	99.352
Nonpolar	ASN 101 - LYS 254	TA02 - TB02	99.314
Nonpolar	LYS 394 - PRO 348	TA02 - TB02	99.014
Nonpolar	THR 179 - LEU 248	TA02 - TB02	98.962
Nonpolar	PHE 404 - ILE 347	TA02 - TB02	98.852
Nonpolar	VAL 182 - VAL 257	TA02 - TB02	98.295
Nonpolar	MET 398 - PRO 348	TA02 - TB02	98.271
Nonpolar	GLU 220 - LYS 326	TA02 - TB02	97.909
Nonpolar	ALA 100 - ARG 253	TA02 - TB02	97.867
Nonpolar	LEU 397 - TRP 346	TA02 - TB02	97.043
Nonpolar	LYS 401 - PHE 262	TA02 - TB02	96.776
Nonpolar	HIS 406 - PRO 263	TA02 - TB02	96.676
Nonpolar	SER 178 - LYS 352	TA02 - TB02	96.557
Nonpolar	PRO 175 - LYS 352	TA02 - TB02	94.085
Nonpolar	HIS 406 - VAL 260	TA02 - TB02	92.538
Nonpolar	ARG 215 - GLU 330	TA02 - TB02	92.009
Nonpolar	TRP 407 - ALA 256	TA02 - TB02	91.785
Nonpolar	GLU 97 - ARG 253	TA02 - TB02	91.766
Nonpolar	ARG 214 - LYS 326	TA02 - TB02	91.709
Nonpolar	ALA 100 - LYS 254	TA02 - TB02	91.300
Nonpolar	MET 398 - ILE 347	TA02 - TB02	91.242

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	ALA 180 - ASN 258	TA02 - TB02	90.219
Nonpolar	LEU 397 - PRO 348	TA02 - TB02	89.419
Nonpolar	ASP 98 - ARG 253	TA02 - TB02	88.895
Nonpolar	TRP 407 - VAL 257	TA02 - TB02	88.142
Nonpolar	PRO 175 - ASN 349	TA02 - TB02	88.085
Nonpolar	VAL 181 - LYS 352	TA02 - TB02	87.857
Nonpolar	HIS 406 - PRO 261	TA02 - TB02	87.280
Nonpolar	PHE 404 - VAL 257	TA02 - TB02	87.142
Nonpolar	ARG 214 - GLU 330	TA02 - TB02	87.133
Nonpolar	LYS 401 - TRP 346	TA02 - TB02	86.123
Nonpolar	ALA 403 - TRP 346	TA02 - TB02	82.375
Nonpolar	HIS 406 - PHE 262	TA02 - TB02	82.113
Nonpolar	ARG 221 - VAL 355	TA02 - TB02	81.899
Nonpolar	TYR 224 - GLN 247	TA02 - TB02	81.461
Nonpolar	ARG 402 - PHE 262	TA02 - TB02	80.828
Nonpolar	GLU 71 - MET 1	TA02 - TB02	80.799
Nonpolar	PHE 404 - PRO 261	TB02 - TA03	100.000
Nonpolar	ASN 101 - ASN 258	TB02 - TA03	99.800
Nonpolar	GLY 100 - GLU 254	TB02 - TA03	99.586
Nonpolar	GLU 71 - ARG 2	TB02 - TA03	99.457
Nonpolar	TRP 407 - VAL 260	TB02 - TA03	99.438
Nonpolar	ASN 101 - LYS 352	TB02 - TA03	98.319
Nonpolar	ASP 179 - LYS 352	TB02 - TA03	98.295

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GLY 100 - THR 257	TB02 - TA03	96.509
Nonpolar	THR 180 - ASN 258	TB02 - TA03	96.252
Nonpolar	GLY 100 - THR 253	TB02 - TA03	96.219
Nonpolar	VAL 181 - PRO 348	TB02 - TA03	95.366
Nonpolar	ALA 397 - TRP 346	TB02 - TA03	94.505
Nonpolar	HIS 406 - PRO 263	TB02 - TA03	94.104
Nonpolar	MET 398 - TRP 346	TB02 - TA03	94.062
Nonpolar	PHE 404 - THR 257	TB02 - TA03	90.214
Nonpolar	SER 178 - GLY 350	TB02 - TA03	89.933
Nonpolar	GLN 394 - PRO 348	TB02 - TA03	89.161
Nonpolar	ALA 403 - PRO 261	TB02 - TA03	88.490
Nonpolar	ARG 401 - TRP 346	TB02 - TA03	85.952
Nonpolar	ARG 401 - VAL 440	TB02 - TA03	85.833
Nonpolar	MET 398 - PRO 348	TB02 - TA03	85.766
Nonpolar	ALA 403 - TYR 262	TB02 - TA03	85.537
Nonpolar	ASN 101 - THR 257	TB02 - TA03	85.380
Nonpolar	ASN 101 - GLU 254	TB02 - TA03	84.314
Nonpolar	PRO 184 - PRO 348	TB02 - TA03	81.728
Nonpolar	SER 97 - ARG 2	TB02 - TA03	80.732
Nonpolar	PHE 404 - PRO 261	TA03 - TB03	100.000
Nonpolar	ALA 100 - LYS 254	TA03 - TB03	99.995
Nonpolar	ASP 98 - LYS 254	TA03 - TB03	99.971
Nonpolar	TRP 407 - VAL 260	TA03 - TB03	99.929

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	VAL 181 - ASN 258	TA03 - TB03	99.643
Nonpolar	PHE 404 - ILE 347	TA03 - TB03	99.290
Nonpolar	GLU 71 - LYS 254	TA03 - TB03	99.148
Nonpolar	LEU 397 - TRP 346	TA03 - TB03	98.038
Nonpolar	ARG 221 - ASP 329	TA03 - TB03	97.271
Nonpolar	LYS 401 - PHE 262	TA03 - TB03	96.100
Nonpolar	ALA 180 - ASN 258	TA03 - TB03	96.086
Nonpolar	MET 398 - PRO 348	TA03 - TB03	95.881
Nonpolar	VAL 181 - LYS 352	TA03 - TB03	95.781
Nonpolar	SER 178 - LYS 352	TA03 - TB03	94.738
Nonpolar	ARG 221 - LYS 326	TA03 - TB03	94.605
Nonpolar	HIS 406 - PRO 263	TA03 - TB03	94.352
Nonpolar	HIS 406 - VAL 260	TA03 - TB03	94.162
Nonpolar	ASN 101 - LYS 254	TA03 - TB03	93.785
Nonpolar	VAL 182 - VAL 257	TA03 - TB03	93.700
Nonpolar	PHE 404 - VAL 257	TA03 - TB03	92.576
Nonpolar	GLU 220 - LYS 326	TA03 - TB03	91.642
Nonpolar	GLN 176 - LEU 333	TA03 - TB03	90.719
Nonpolar	TRP 407 - VAL 257	TA03 - TB03	88.118
Nonpolar	TRP 407 - ALA 256	TA03 - TB03	87.990
Nonpolar	LEU 397 - PRO 348	TA03 - TB03	86.523
Nonpolar	LYS 394 - PRO 348	TA03 - TB03	85.490
Nonpolar	HIS 406 - PRO 261	TA03 - TB03	84.656

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	ALA 403 - TRP 346	TA03 - TB03	83.161
Nonpolar	PRO 175 - ASN 349	TA03 - TB03	82.104
Nonpolar	LYS 401 - TRP 346	TA03 - TB03	81.056
Nonpolar	ALA 403 - PRO 261	TA03 - TB03	80.113
Nonpolar	GTP 1 - GLY 146	GTP - TA00	100.000
Nonpolar	GTP 1 - THR 145	GTP - TA00	100.000
Nonpolar	GTP 1 - GLY 143	GTP - TA00	100.000
Nonpolar	GTP 1 - ALA 12	GTP - TA00	100.000
Nonpolar	GTP 1 - GLN 11	GTP - TA00	100.000
Nonpolar	GTP 1 - ASN 228	GTP - TA00	99.995
Nonpolar	GTP 1 - THR 179	GTP - TA00	99.786
Nonpolar	GTP 1 - ASP 69	GTP - TA00	99.429
Nonpolar	GTP 1 - ALA 100	GTP - TA00	99.205
Nonpolar	GTP 1 - ALA 99	GTP - TA00	98.643
Nonpolar	GTP 1 - GLY 10	GTP - TA00	98.090
Nonpolar	GTP 1 - TYR 224	GTP - TA00	97.952
Nonpolar	GTP 1 - VAL 177	GTP - TA00	96.695
Nonpolar	GTP 1 - ASN 206	GTP - TA00	95.466
Nonpolar	GTP 1 - ASP 98	GTP - TA00	95.133
Nonpolar	GTP 1 - SER 140	GTP - TA00	93.804
Nonpolar	GTP 1 - GLN 15	GTP - TA00	92.504
Nonpolar	GTP 1 - GLY 144	GTP - TA00	90.395
Nonpolar	GTP 1 - ILE 171	GTP - TA00	82.833

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GDP 1 - GLY 143	GDP - TB00	99.962
Nonpolar	GDP 1 - ASN 228	GDP - TB00	99.700
Nonpolar	GDP 1 - TYR 224	GDP - TB00	98.357
Nonpolar	GDP 1 - GLU 183	GDP - TB00	92.085
Nonpolar	GDP 1 - CYS 12	GDP - TB00	86.214
Nonpolar	GDP 1 - SER 140	GDP - TB00	85.147
Nonpolar	GTP 2 - THR 145	GTP - TA01	100.000
Nonpolar	GTP 2 - GLN 11	GTP - TA01	100.000
Nonpolar	GTP 2 - ASN 228	GTP - TA01	99.995
Nonpolar	GTP 2 - ALA 12	GTP - TA01	99.986
Nonpolar	GTP 2 - ASP 69	GTP - TA01	99.843
Nonpolar	GTP 2 - GLY 143	GTP - TA01	99.767
Nonpolar	GTP 2 - GLY 146	GTP - TA01	97.852
Nonpolar	GTP 2 - TYR 224	GTP - TA01	97.562
Nonpolar	GTP 2 - GLY 10	GTP - TA01	89.452
Nonpolar	GTP 2 - GLN 15	GTP - TA01	87.018
Nonpolar	GDP 2 - ASN 228	GDP - TB01	100.000
Nonpolar	GDP 2 - GLY 143	GDP - TB01	99.981
Nonpolar	GDP 2 - THR 145	GDP - TB01	99.890
Nonpolar	GDP 2 - GLY 144	GDP - TB01	99.819
Nonpolar	GDP 2 - GLU 183	GDP - TB01	99.686
Nonpolar	GDP 2 - ASN 206	GDP - TB01	99.095
Nonpolar	GDP 2 - ASP 179	GDP - TB01	99.081

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GDP 2 - TYR 224	GDP - TB01	97.419
Nonpolar	GDP 2 - CYS 12	GDP - TB01	95.862
Nonpolar	GDP 2 - VAL 177	GDP - TB01	95.833
Nonpolar	GDP 2 - SER 178	GDP - TB01	94.166
Nonpolar	GTP 3 - GLY 146	GTP - TA02	100.000
Nonpolar	GTP 3 - THR 145	GTP - TA02	100.000
Nonpolar	GTP 3 - GLY 143	GTP - TA02	100.000
Nonpolar	GTP 3 - ALA 12	GTP - TA02	100.000
Nonpolar	GTP 3 - GLN 11	GTP - TA02	100.000
Nonpolar	GTP 3 - GLY 144	GTP - TA02	99.976
Nonpolar	GTP 3 - ASP 69	GTP - TA02	99.976
Nonpolar	GTP 3 - ASN 101	GTP - TA02	99.971
Nonpolar	GTP 3 - ASN 228	GTP - TA02	99.386
Nonpolar	GTP 3 - GLY 10	GTP - TA02	98.338
Nonpolar	GTP 3 - TYR 224	GTP - TA02	98.033
Nonpolar	GTP 3 - SER 140	GTP - TA02	95.762
Nonpolar	GTP 3 - ALA 99	GTP - TA02	90.200
Nonpolar	GTP 3 - SER 178	GTP - TA02	89.219
Nonpolar	GTP 3 - ASN 206	GTP - TA02	88.071
Nonpolar	GTP 3 - GLN 15	GTP - TA02	82.094
Nonpolar	GDP 3 - ASN 228	GDP - TB02	100.000
Nonpolar	GDP 3 - ASN 206	GDP - TB02	99.995
Nonpolar	GDP 3 - TYR 224	GDP - TB02	99.643

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GDP 3 - GLY 143	GDP - TB02	99.629
Nonpolar	GDP 3 - SER 140	GDP - TB02	98.967
Nonpolar	GDP 3 - PRO 173	GDP - TB02	87.942
Nonpolar	GDP 3 - VAL 171	GDP - TB02	86.790
Nonpolar	GDP 3 - CYS 12	GDP - TB02	80.070
Nonpolar	GTP 4 - GLY 146	GTP - TA03	100.000
Nonpolar	GTP 4 - THR 145	GTP - TA03	100.000
Nonpolar	GTP 4 - GLY 144	GTP - TA03	100.000
Nonpolar	GTP 4 - GLY 143	GTP - TA03	100.000
Nonpolar	GTP 4 - ASN 101	GTP - TA03	100.000
Nonpolar	GTP 4 - ALA 12	GTP - TA03	100.000
Nonpolar	GTP 4 - GLN 11	GTP - TA03	100.000
Nonpolar	GTP 4 - ASN 228	GTP - TA03	99.995
Nonpolar	GTP 4 - ASP 69	GTP - TA03	99.900
Nonpolar	GTP 4 - GLU 183	GTP - TA03	99.771
Nonpolar	GTP 4 - TYR 224	GTP - TA03	98.000
Nonpolar	GTP 4 - SER 140	GTP - TA03	97.219
Nonpolar	GTP 4 - ASN 206	GTP - TA03	93.857
Nonpolar	GTP 4 - GLY 10	GTP - TA03	93.185
Nonpolar	GTP 4 - SER 178	GTP - TA03	84.837
Nonpolar	GTP 4 - ALA 99	GTP - TA03	84.618
Nonpolar	GTP 4 - VAL 177	GTP - TA03	84.061
Nonpolar	GDP 4 - GLY 143	GDP - TB03	99.981

Table 4.6: Continued

Contact Type	Contact	Domain	% Occupancy
Nonpolar	GDP 4 - ASN 228	GDP - TB03	99.976
Nonpolar	GDP 4 - CYS 12	GDP - TB03	99.910
Nonpolar	GDP 4 - GLY 144	GDP - TB03	99.895
Nonpolar	GDP 4 - GLN 11	GDP - TB03	98.638
Nonpolar	GDP 4 - TYR 224	GDP - TB03	96.924
Nonpolar	GDP 4 - THR 145	GDP - TB03	96.733
Nonpolar	GDP 4 - SER 140	GDP - TB03	95.976
Nonpolar	GDP 4 - ASN 206	GDP - TB03	92.666
Nonpolar	GDP 4 - GLU 183	GDP - TB03	91.247
Nonpolar	GDP 4 - SER 178	GDP - TB03	89.023
Nonpolar	GDP 4 - GLN 15	GDP - TB03	82.323
End of Table 4.6			