ANALYSIS OF PSEUDO-SYMMETRY IN PROTEIN OLIGOMERS AND ITS CORRELATION WITH PROTEIN DYNAMICS

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TABLE OF CONTENTS

Page

LIST OF TABLES

LIST OF FIGURES

Figure Page

SYMBOLS

Å	Resolution in Angstrom
B	B-Factor
B_{min}	Minimum B-Factor
B_{max}	Maximum B-Factor
B_{norm}	Normalized B-Factor

ABBREVIATIONS

AI	Assembly Index
AI_CA	Assembly Index for CA atoms
AI_CB	Assembly Index for CB atoms
BF/OS	OS and B-Factor Correlation
BF/SI	SI and B-Factor Correlation
BF/AI	AI and B-Factor Correlation
CA	Carbon alpha
CB	Carbon Beta
D	Domain
MBF	Mean B-Factor
OS	Off-Symmetry
OS_CA	Off-Symmetry for CA atoms
OS_CB	Off-Symmetry for CB atoms
RBF	B-Factor Range
RMSB	Root Mean Square Deviation
SI	Structure Index
SI_CA	Structure Index for CA atoms
SI_CB	Structure Index for CB atoms

ABSTRACT

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Symmetry is a feature that can be noticed almost anywhere around us. Animals, for example, have bilateral symmetry whereas flowers have a rotational symmetry. Proteins are complex systems that also exhibit this property as a rule but there is a disturbance in it that prevents it from being perfectly symmetrical. Even homo-oligomers that are made of identical subunits are not exempt from this. In this paper, we focused on protein homo-dimers and homo-trimers and we introduced off-symmetry(OS) to quantify how much a protein complex is off from perfect symmetry. Furthermore, we decomposed off-symmetry into two aspects namely structure index (SI) that measures structural difference and assembly index (AI) that measures assembly difference. We found in most cases, the major contributor to OS is SI in dimers and AI in trimers. In addition, we found that the SI and in turn OS contributed by each residue is positively correlated with their B factors, which indicates that protein flexibility and mobility may contribute to the off-symmetry of protein oligomers.

1. INTRODUCTION

Assembly of specific number of monomer units make oligomer complexes and these units can either be identical or non-identical forming a homo-oligomer and hetero-oligomer respectively. Protein tertiary and quaternary structures possess symmetry as a feature attributed to folding, stability, etc. According to the RCSB, complexes are symmetrical if identical subunits superpose with their symmetry related copies within 7Å RMSD. In this paper, we focus on pseudo-symmetry in homodimers and homotrimers.

Various algorithms have been developed to detect symmetry which use structural alignment of secondary elements. SymD is one such algorithm which performs different transformations like rotations and translations and measures the symmetry by checking if any of these transformations results in a large number of superimposed residues between the original and transformed structures [1]. CE-Symm is another algorithm that detects internal symmetry using the Combinatorial Extension (CE) algorithm to perform protein structure alignment and using those results to detect symmetry [2]. It can easily identify structural repeats like rotational symmetry by using features like Root Mean Square Deviation (RMSD), TM-Score and Z-score. Even though these algorithms detect symmetry, they are not designed to quantify protein symmetry.

Although proteins are considered to be symmetric, not many of them are perfectly symmetrical. Continuous Symmetry Measures (CSM) is one of those tools that can be used to quantify symmetry. CSM evaluates the degree of symmetries like mirror, rotation, inversion and improper rotation of a structure [3] [4]. It defines the symmetry of a structure to be the minimal distance that the vertices of the structure have to undergo in order for it to attain the desired symmetry which they define formally as "the normalized root-mean-square deviation from the closest structure with

desired symmetry". It does not deal with preset structures, but evaluates distance to the desired symmetry. Given a structure with N vertices, the tool searches for the vertices of the nearest perfectly G-symmetric object (G is the specific symmetry group) and calculates the distance to it. This tool finds the issue of deviation from perfect symmetry. The causes for a disturbance like this is still being researched upon especially in homo-oligomers that constitute identical chains.

1.1 Structural and Assembly Equivalence

As already mentioned, the parameters that contribute to protein symmetry are structural and assembly equivalence and these are explained by taking homodimers as an example. A homodimer contains two subunits for which a two-fold axis can be determined. A homodimer with perfect two-fold symmetry has two chains that have the same 3D structure and are aligned correlatively along the axis in 3D space. To explain structural and assembly equivalence, consider the fig. 1.1 below. Fig. 1.1A shows that the protein is an example for perfect symmetry. In fig. 1.1B, the chains are structurally in-equivalent even though they are assembled equivalently along the axis. In fig. 1.1C, even though there is structural equivalence there is no assembly equivalence. These two factors contribute to off-symmetry.

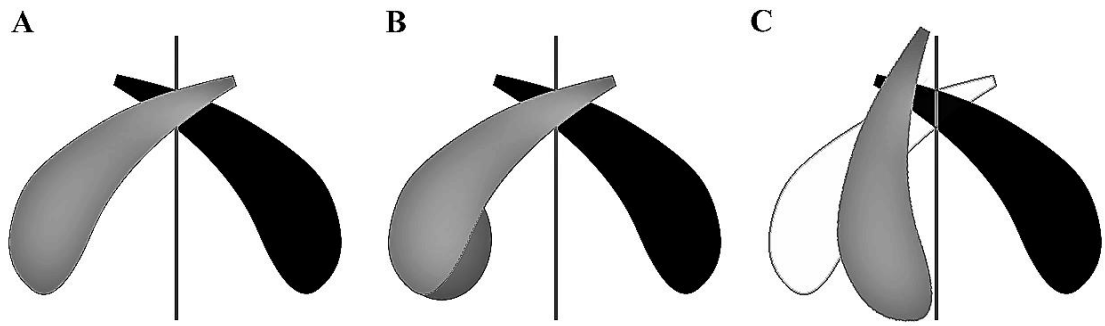

Fig. 1.1.: Schematic representation of Homodimers.(A) Shows two chains in black and gray in perfect two-fold symmetry.(B) The two chains are not in perfect symmetry because of structural in-equivalence depicted in dark gray even though there is assembly equivalence. (C) The two chains are not in perfect symmetry because there is structural equivalence but they are not aligned perfectly in 3-D space.

1.2 Rotational Symmetry in Proteins

Protein complexes possess the property of being rotationally symmetrical. Dimers have C2 symmetry, trimers have C3 symmetry and some tetramers have C4 symmetry [5] [6]. When oligomers are rotated by a said degree along their axis of symmetry, the resultant structure is similar to the original.

Dimers having chains, namely, A and B when rotated along the two-fold axis by 180 degrees produce a structure similar to the original with the chains' positions interchanged to get A' and B'. Trimers, on the other hand, having three subunits are rotated along the three-fold axis by 120° clockwise twice to get back the original structure. Off Symmetry(OS) is computed by comparing the resultant structures with the original. OS, SI and AI are explained below by taking trimers as an example.

Perfect symmetry in trimers exists when the chains are assembled in the form of an equilateral triangle and rotation of the trimer by 120° clockwise about its 3-fold axis produces a structure similar to the original as shown in fig 1.2.

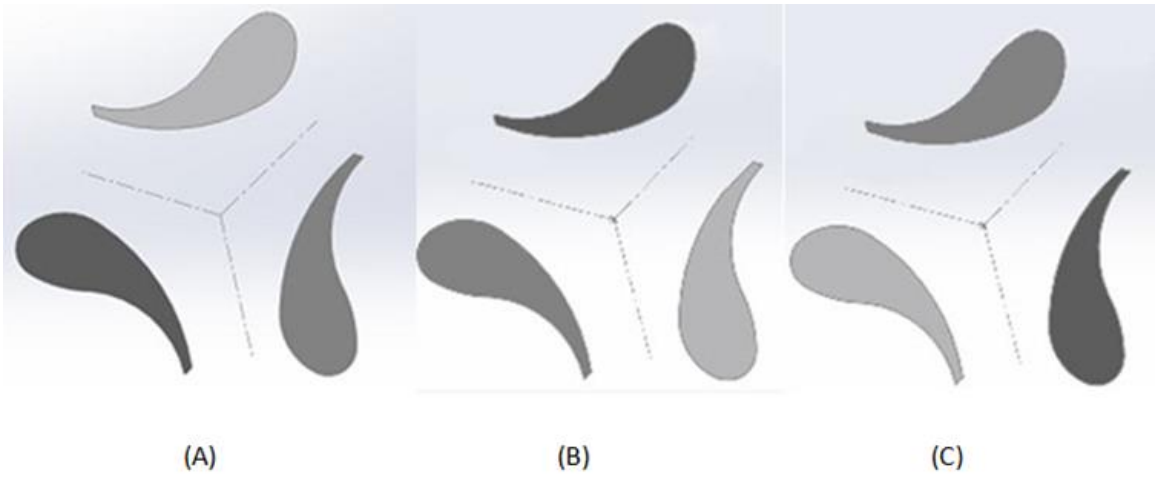

Fig. 1.2.: (A) Depicts the trimer with its subunits assembled in the form of an equilateral triangle with the angle between each being 120 degrees.(B) Depicts the resultant structure when the (A) is rotated 120 degrees clockwise about the axis normal to the Z-plane.(C) Depicts the resultant structure when (A) is rotated 240 degrees clockwise about the axis normal to the Z-plane. In the case of pure symmetrical trimer, the resultant structures are identical to the original one.

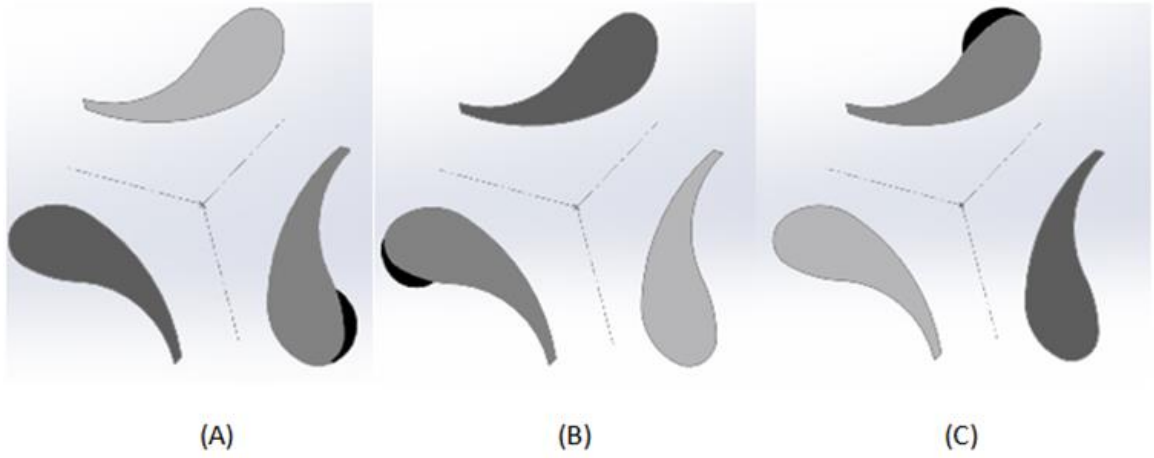

Fig. 1.3.: (A) Depicts a trimer with one of the subunits as structurally different(Shaded black portion) from the others.(B) Depicts the resultant structure when the (A) is rotated 120 degrees clockwise about the axis normal to the Z-plane.(C) Depicts the resultant structure when (A) is rotated 240 degrees clockwise about the axis normal to the Z-plane. In this case, the resultant structures are different from the original one and off-symmetry is introduced purely by structure difference.

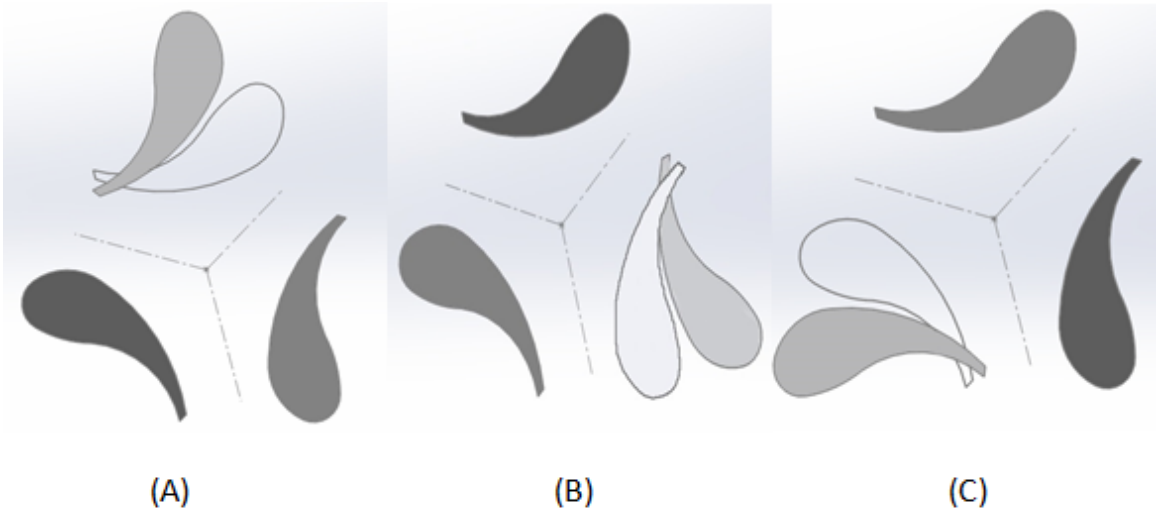

Fig. 1.4.: (A) Depicts a trimer with one of the subunit misaligned from its equivalent position indicated by open shape.(B) Depicts the resultant structure when (A) is rotated 120 degrees clockwise about the axis normal to the Z-plane.(C) Depicts the resultant structure when (A) is rotated 240 degrees clockwise about the axis normal to the Z-plane. In this case, the resultant structures are different from the original one and the off-symmetry is introduced purely by assembly difference.

Fig. 1.3 and fig. 1.4. show how structure and assembly difference contribute to off-symmetry, respectively. In reality, the off-symmetry of protein oligomers are simultaneously contributed by both sources. How we treat and measure the contribution from structure and assembly difference separately will be described shortly.

2. CALCULATING OFF-SYMMETRY, STRUCTURE INDEX AND ASSEMBLY INDEX WITHOUT USING ROTATIONAL SYMMETRY

Prior to using rotational symmetry, we had come up with a method to compute OS, SI and AI in homodimers. The approach has been explained below along with reasons as to why this method is not feasible.

Off-Symmetry A homodimer is perfectly symmetrical if the distance between the mth atom in chain A and the nth atom in chain B is equal to the distance between the nth atom in chain A and mth atom in chain B, i.e, A_mB_n=A_nB_m and m is not equal to n.

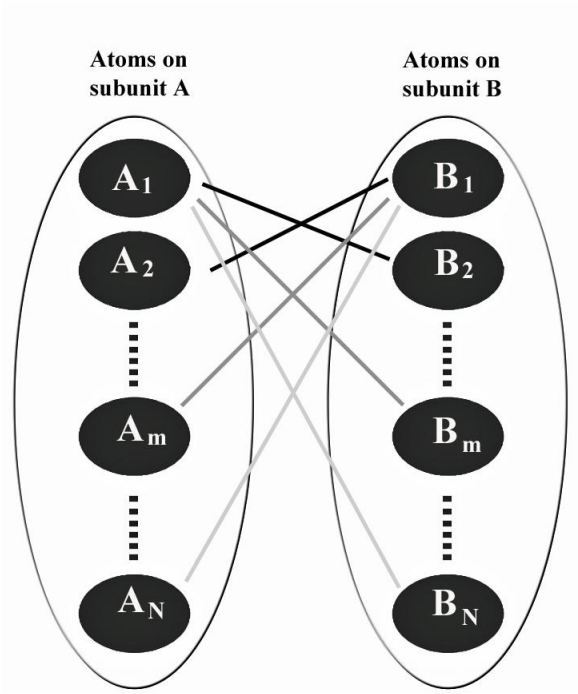

Fig. 2.1.: Off-Symmetry in Homodimers

In order to calculate the Off-Symmetry,we assume there are N atoms in each chain/subunit and the following formula was defined:

$$OS = \frac{\sum_{n,m=1}^{N} |A_{\mathrm{m}} B_{\mathrm{n}} - B_{\mathrm{m}} A_{\mathrm{n}}|}{N(N-1)/2} \tag{2.1}$$

where m≤N, n≤N and m≠n.

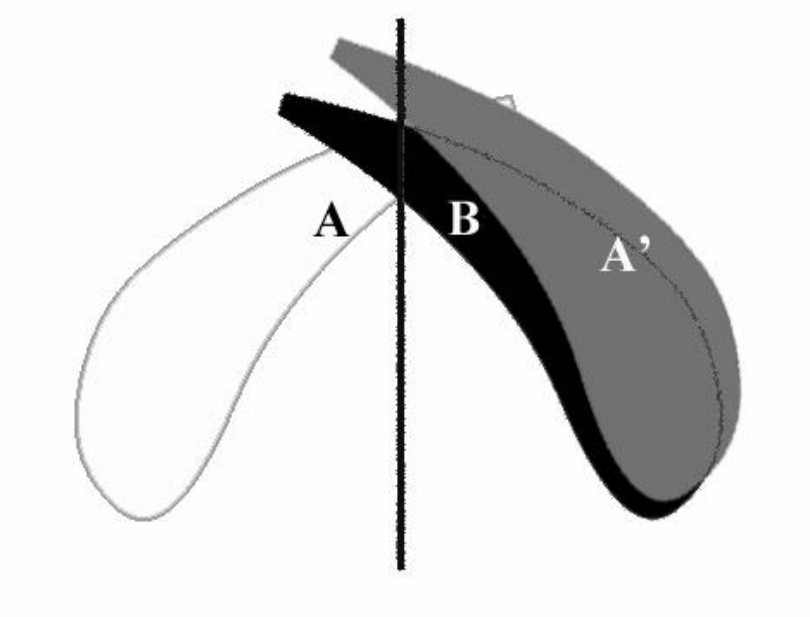

Fig. 2.2.: Chain A is aligned with chain B to get A' and SI is calculated based on the paired distances between the atoms in A' and B. AI is based on the paired distances between the atoms in A' and the original chain A.

Structure Index It is one of the parameters that constitutes Off-Symmetry and is calculated by performing a least-squares fitting in the two subunits by moving the first set of CA atoms onto the second set of CA atoms by using the Chimera module and is defined as follows:

$$SI = \frac{\sum_{n,m=1}^{N} |A'_{\mathrm{m}} B_{\mathrm{n}} - B_{\mathrm{m}} A'_{\mathrm{n}}|}{N(N-1)/2} \tag{2.2}$$

where m≤N, n≤N and m≠n. Here, A' indicates the chain that is aligned with chain B as shown in Fig.2.2.

Assembly Index It is the second parameter that constitutes Off-Symmetry and defined as follows:

$$AI = \frac{\sum_{n,m=1}^{N} |A_{\mathrm{m}} A''_{\mathrm{n}} - A''_{\mathrm{m}} A_{\mathrm{n}}|}{N(N-1)/2} \tag{2.3}$$

where m≤N, n≤N and m≠n.

Although this is a valid method, there are a few drawbacks to it. This approach cannot be applied to homo-oligomers like homotrimers because they have a 3-fold axis of symmetry. Also, the computation that is needed to calculate the OS, SI and AI is complicated and there are possibilities for the occurrence of normalization issues. These drawbacks gave way to using rotational symmetry to compute off-symmetry that can be applied to both dimers and trimers and deals with much simpler computation.

3. USING ROTATIONAL SYMMETRY TO CALCULATE OFF-SYMMETRY, STRUCTURE INDEX AND ASSEMBLY INDEX

This approach to finding Off-Symmetry is simple and uses the property of protein complexes being rotationally symmetrical. Homodimers have a two-fold axis of symmetry and therefore, fall into the cyclic group of order 2, i.e., C_2. A 180° rotation about the axis produces a structure similar to the first one with the position of the chains interchanged. Homotrimers , on the other hand belong to the C3 group and have a three-fold axis and hence are rotated 120° and 240° clockwise to get two distinct resultant structures that will be compared with the original.

The following steps are followed to find OS, SI and AI:

1. Translate the protein such that the center of mass coincides with the origin and find the axis of symmetry.

2. Rotate the homodimer by 180° along the axis of symmetry. In case of homotrimers, rotate the protein by 120° twice along the axis of symmetry.

3. Find the Euclidean distance between the equivalent atoms in the original and the rotated structures to compute OS. The equivalent atoms as a whole can be all atoms or CA or CB atoms or etc, depending on the study.

4. Structurally align the chains in the proteins and calculate the Euclidean distance between the equivalent atom pairs in the aligned structure and the original structure to compute SI. Similarly, the equivalent atoms to be investigated can be all atoms or CA or CB atoms or etc, depending on the study, but has to be consistent with the calculation of OS.

5. Structurally align the chains in the proteins and calculate the Euclidean distance between the equivalent atom pairs in the aligned structure and the rotated structure to compute AI. Similarly, the equivalent atoms to be investigated can be all atoms or CA or CB atoms or etc, depending on the study, but has to be consistent with the calculation of OS.

Each of these steps is explained in detail below.

Protein Data Set Homodimer and homotrimer proteins were downloaded from the RCSB Protein Data Bank (www.rcsb.org) with X-Ray resolution value in between 0.0Å and 1.5Å and a 30% sequence identity as of August 2015. For dimers, the number of chains of both biological assembly and asymmetric unit is set to be 2. In case of trimers, the number of chains of both biological assembly and asymmetric unit is set to be 3. The proteins were examined for unequal number of atoms between the chains and atoms that do not exist in every chain of the protein complex is excluded in calculating OS, SI and AI parameters. All nonstandard residues i.e. ions, water were also excluded in the calculations. We compare the OS, SI and AI for the CA and CB atoms in the protein.

3.1 Calculating OS, SI and AI in Homodimers

3.1.1 Finding the Two Fold Axis

All homodimers are translated from their initial position such that their center of mass coincides with the origin. New pdb files are generated and this is used as an input to find the two-fold symmetry. We then use Chimera to calculate the two-fold axis of the homodimer. Two models of the same protein are opened and the following commands are executed:

```
mm #0:.A:.B #1:.B:.A pair ss
measure rotation #0 #1
```

The Reply Log gives the direction of the axis and this is used for rotation of the dimer.

3.1.2 Off-Symmetry

In order to calculate the off-symmetry, the homodimer with chains A and B is rotated by 180° using Chimera, along the two-fold axis to get A'(180) and B'(180) in the second structure such that A'(180) is in the position of B in the original structure and B'(180) is in the position of A in the original structure. Assuming there are N atoms in each subunit, Off-Symmetry is calculated by using the following formula:

$$OS = \frac{\sum_{n=1}^{N}(|A'_{\mathrm{n}}(180)B_{\mathrm{n}}| + |B'_{\mathrm{n}}(180)A_{\mathrm{n}}|)}{2N} \tag{3.1}$$

The above formula computes absolute distance between each pair of atoms in every residue. The atoms to be included in the computation can be all atoms, CA or any group of atoms of interest.

3.1.3 Structure Index

Structure Index is calculated by aligning the atoms of chain A with the atoms in chain B using Chimera's match module to get A" and atoms of chain B with the atoms in chain A to get B" and calculating the distance between the paired atoms in chain A" and chain B in the original structure and chain B" and chain A in the original structure using the following formula:

$$SI = \frac{\sum_{n=1}^{N}(|A''_{\mathrm{n}}B_{\mathrm{n}}| + |B''_{\mathrm{n}}A_{\mathrm{n}}|)}{2N} \tag{3.2}$$

Similarly, the atoms to be included in the computation cab be all atoms, CA or any group of atoms of interest.

3.1.4 Assembly Index

Assembly Index is calculated by aligning the atoms of interest in chain A with those atoms in chain B using Chimera's match module to get A" and atoms of chain B with those atoms in chain A and calculating the distance between the paired atoms in chain A" and chain A'(180) in the second structure and chain B" and chain B'(180) in the second structure using the following formula:

$$AI = \frac{\sum_{n=1}^{N}(|A''_{\mathrm{n}}A'_{\mathrm{n}}(180)| + |B''_{\mathrm{n}}B'_{\mathrm{n}}(180)|)}{2N} \tag{3.3}$$

Similarly, the atoms to be included in the computation can be all atoms, CA or any group of atoms of interest.

3.2 Calculating OS, SI and AI in Homotrimers

3.2.1 Finding the Three Fold Axis

All homotrimers are translated from their initial position such that their center of mass coincides with the origin (Refer to B.Translate.py). The axis for a trimer is normal to the trimer's plane and this axis is found by using Chimera and then it is then rotated by 120° and 240° about the center along the axis of symmetry.

3.2.2 Off-Symmetry

The homotrimer is rotated 120° along the three-fold axis in the clockwise direction to generate C'(120), B'(120) and A'(120) that are in the position equivalent to A, C and B of the original structure (fig.1.3B and fig.1.4B). The distance between the atoms in the corresponding chains are compared and off-symmetry (120) is calculated as follows:

$$OS(120) = \frac{\sum_{n=1}^{N}(|A_{\mathrm{n}}C'_{\mathrm{n}}(120)| + |C_{\mathrm{n}}B'_{\mathrm{n}}(120)| + |B_{\mathrm{n}}A'_{\mathrm{n}}(120)|)}{3N} \tag{3.4}$$

The same procedure is followed when the homotrimer is rotated by another 120° (total of 240°) to generate B'(240), C'(240) and A'(240) that are in the position

equivalent to A, B and C of the original structure, respectively (fig.1.3C and fig.1.4C) and the following formula is used:

$$OS(240) = \frac{\sum_{n=1}^{N}(|A_{\mathrm{n}}B'_{\mathrm{n}}(240)| + |C_{\mathrm{n}}A'_{\mathrm{n}}(240)| + |B_{\mathrm{n}}C'_{\mathrm{n}}(240)|)}{3N} \tag{3.5}$$

Once the OS(120) and OS(240) is found, the mean value of the two gives us the final OS value.

$$OS = \frac{OS(120) + OS(240)}{2} \tag{3.6}$$

3.2.3 Structure Index

Structure Index is computed by aligning chain A with B to get A", B with C to get B", C with A to get C" using the Chimera match module in the position equivalent to A, B and C of the original structure(fig.1.4A and fig.1.4B). The distance between the atoms in the corresponding chains are compared and SI(120) is calculated as follows:

$$SI(120) = \frac{\sum_{n=1}^{N}(|A''_{\mathrm{n}}B_{\mathrm{n}}| + |B''_{\mathrm{n}}C_{\mathrm{n}}| + |C''_{\mathrm{n}}A_{\mathrm{n}}|)}{3N} \tag{3.7}$$

The same procedure is followed for 240° rotation, chain A is aligned with C to get A", C with B to get C" and B with A to get B" in the position equivalent to C, B and A of the original structure(fig.1.4A and fig.1.4C) and the SI(240) is calculated as follows:

$$SI(240) = \frac{\sum_{n=1}^{N}(|A''_{\mathrm{n}}C_{\mathrm{n}}| + |B''_{\mathrm{n}}A_{\mathrm{n}}| + |C''_{\mathrm{n}}B_{\mathrm{n}}|)}{3N} \tag{3.8}$$

Once the SI(120) and SI(240) is found, the mean value of the two gives us the final SI value.

$$SI = \frac{SI(120) + SI(240)}{2} \tag{3.9}$$

3.2.4 Assembly Index

Assembly Index is computed by aligning chain A with B to get A", B with C to get B",C with A to get C" using the Chimera match module in the position equivalent

to A', B' and C' in the rotated structure(fig). The distance between the atoms in the corresponding chains are compared and AI(120) is calculated as follows:

$$AI(120) = \frac{\sum_{n=1}^{N}(|A'_{\mathrm{n}}(120)A''_{\mathrm{n}}| + |B'_{\mathrm{n}}(120)B''_{\mathrm{n}}| + |C'_{\mathrm{n}}(120)C''_{\mathrm{n}}|)}{3N} \tag{3.10}$$

The same procedure is followed for 240° rotation, chain A is aligned with C to get A", C with B to get C" and B with A to get B" in the position equivalent to C, B and A of the original structure(fig.1.4B and fig.1.4C) and the AI(240) is calculated as follows:

$$AI(240) = \frac{\sum_{n=1}^{N}(|A'_{\mathrm{n}}(240)A''_{\mathrm{n}}| + |B'_{\mathrm{n}}(240)B''_{\mathrm{n}}| + |C'_{\mathrm{n}}(240)C''_{\mathrm{n}}|)}{3N} \tag{3.11}$$

Once the AI(120) and AI(240) is found, the mean value of the two gives us the final AI value.

$$AI = \frac{AI(120) + AI(240)}{2} \tag{3.12}$$

4. FACTORS AFFECTING STRUCTURE AND ASSEMBLY INDEX

4.1 Correlation of Off-Symmetry, Structure Index and Assembly Index with B-Factor

By definition, B-factor is the displacement of atoms in the protein structure from their mean position. When an atom is more flexible, the resultant displacement is also larger. When an atom has a high B-Factor it is usually more mobile. We calculated the average OS, SI, AI and B-Factor of every residue in the proteins. From the average B-Factor, normalized B-Factors were computed.

$$B_{\text{norm}} = \frac{B - B_{\text{min}}}{B_{\text{max}} - B_{\text{min}}} \tag{4.1}$$

The correlation between OS and normalized B-Factor and SI and normalized B-Factor and AI and normalized B-Factor for each residue was established and the resultant coefficient was found.

5. RESULTS

5.1 Homodimers

Contribution of Structure and Assembly Index to Off-Symmetry

Structure and assembly index are calculated for 198 protein dimer complexes. In fig.5.1, the protein with pdb code 1e9g is used to illustrate the structures generated to achieve the calculation.

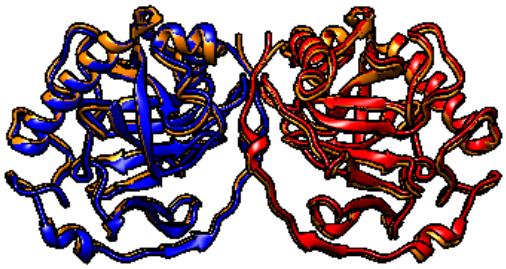

Fig. 5.1.: Off-Symmetry in dimer 1e9g: Structure rotated by 180 degrees and superimposed on the original structure (shown in orange) to generate A' and B'.

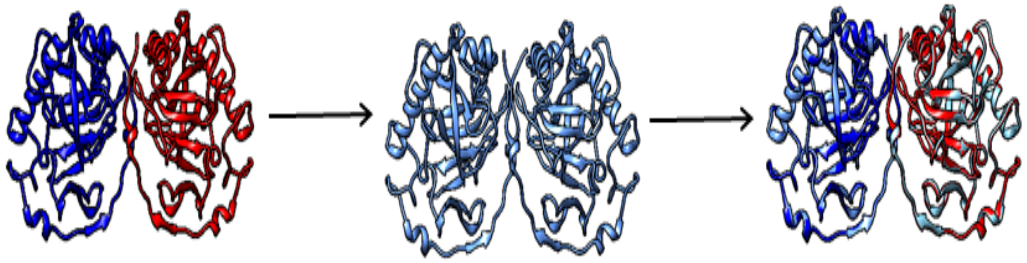

Fig. 5.2.: Structure Index in dimer 1e9g: Structural alignment of chain A with chain B generates A" and chain B with A generates B". The difference between newly generated A" in light blue and chain B in red and generated B" in light blue and chain A in blue produces structure index.

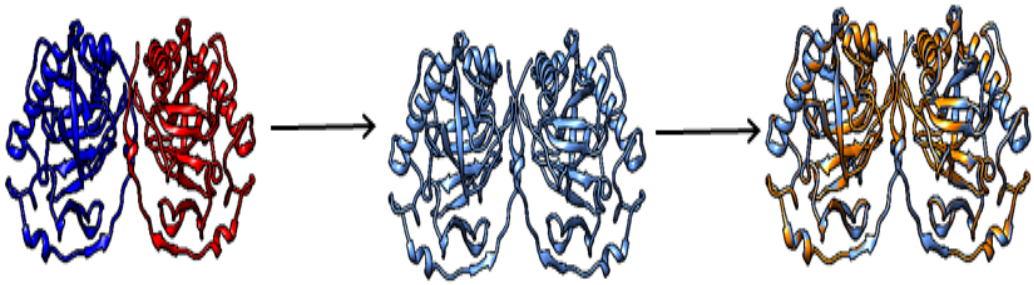

Fig. 5.3.: Assembly Index in dimer 1e9g: Structural alignment of chain A and chain B produces A" and B". The difference between newly generated A" in light blue and chain A' in orange plus generated B" and B' produces assembly index.

We found the total OS, SI, AI, average B-Factor, standard deviation of B-Factor and the B-Factor range of the dimers. The maximum and minimum values for these parameters are below.

Table 5.1.: Minimum and Maximum SI, AI, OS, Mean B-Factor, Stdev B-Factor and B-Factor Range in Homodimers

Min SI	0.08
Max SI	2.51
Min AI	0.02
Max AI	2.95
Min OS	0.08
Max OS	3.07
Min Mean B-Factor	0.14
Max Mean B-Factor	34.88
Min B-Factor Stdev	0.05
Max B-Factor Stdev	11.81
Min B-Factor Range	0.17
Max B-Factor Range	77.07

We calculated the correlation of SI, OS and AI with B-Factor in dimers and have listed the coefficients in table A.1. Specifically, D is the domain of the dimer, BF/OS, BF/SI and BF/AI is the correlation of OS, SI and AI with B-Factor respectively, MBF is the mean B-Factor, SBF is the standard deviation B-Factor, RBF is the B-Factor range, Å is the resolution.

Fig.5.4 shows the contribution of SI and AI to OS by comparing their mean and standard deviation (in the form of a vertical bar). From this figure it can be inferred that SI in general is the major contributor to OS in dimers.

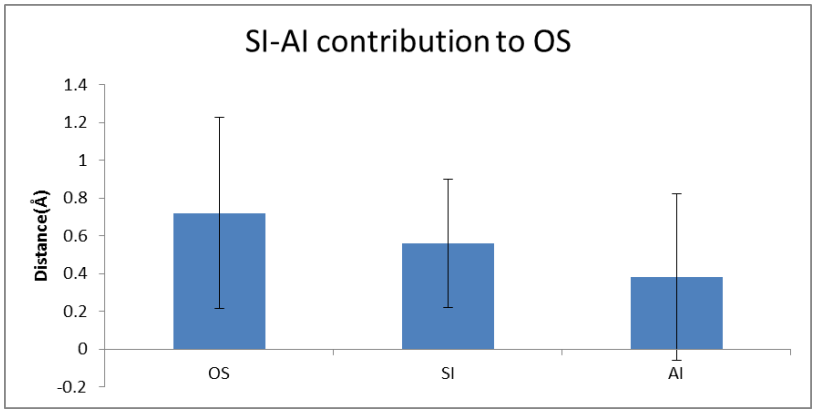

Fig. 5.4.: Contribution of AI and SI to OS in Homodimers

Fig 5.5 shows the comparison of the SI, AI and OS in dimers. While in most cases SI is the major contributor to OS there are cases where AI is the major contributor. Also, for high values of OS it can be noticed that AI can cancel SI and can be considered the only contributor.

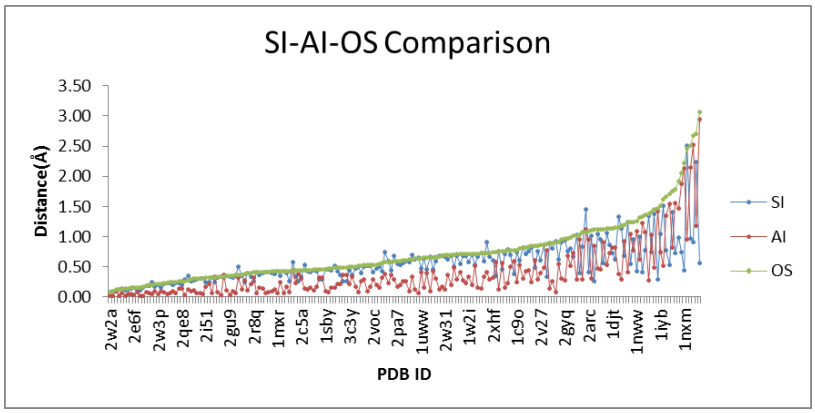

Fig. 5.5.: SI-AI-OS comparison chart for dimers

When OS, AI and SI values were further investigated case by case, there were some interesting trends. As shown in fig. 5.5 when the OS value is low, SI contributes more than AI toward overall OS in most cases. However, as OS value goes higher the contribution from AI starts catching up and plays an important role equivalent or higher than SI. It is worth noting that the OS values in most cases are larger than

individual AI and SI but smaller than the sum of the two. This indicates that AI and SI can partially cancel each other to generate a smaller OS. In some cases, AI values are even higher than OS values, indicating SI to be corrected by AI to generate an overall more symmetrical structure. For example, fig 5.6 shows dimer with pdb code 1uz3, with the original chain B (shown in red), structurally aligned chain A" (shown in light blue) and rotated chain A' (shown in orange). When we look closely at the way the chains are aligned, we can see that the distance between chain B and chain A" is less, so the SI is low. When we look at the distance between chain B and chain A'(which gives us the OS) it is almost equal to the distance between chain A" and chain A' (which gives us AI). Due to this reason, we can say that sometimes there are cases where SI can be canceled out by AI.

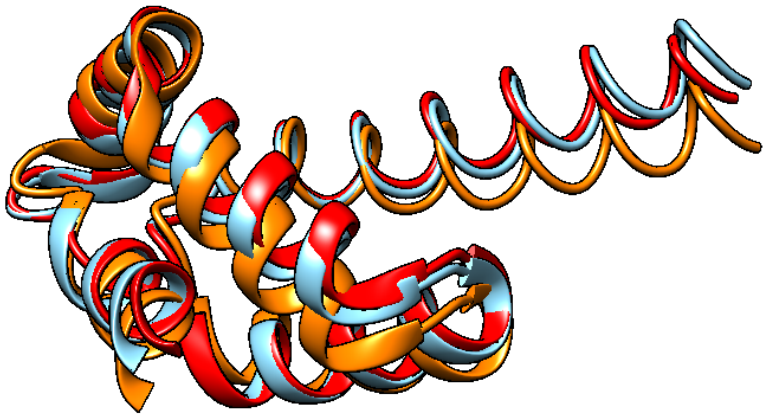

Fig. 5.6.: Dimer 1uz3 with the original chain B (shown in red), structurally aligned chain A"(shown in light blue), rotated chain A'(shown in orange)

Domain-wise comparison of OS, SI and AI In table A.1, the dimers have been grouped based on their domain. Out of the 198 dimers, 163 had 1 domain and 34 had 2 domains. By calculating the average OS, SI and AI for both domains, we found out that the average values of OS, SI and AI for domain 1 was more than the average values for domain 2. Shown in fig 5.6 is a graphical representation of the comparison.

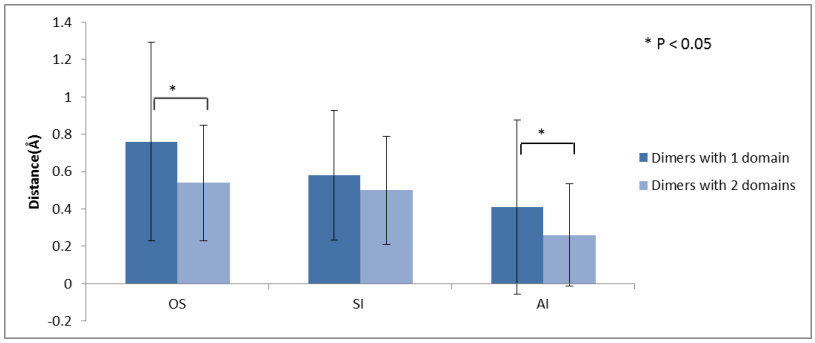

Fig. 5.7.: Domain-wise comparison of OS, SI and AI in Homodimers

For the dimers in the two domains, we conducted a T-test to check if there was a significant difference between the average OS values. Using the null hypothesis, we found that the p-value was 0.0002 and hence there is a significant difference between the average OS in the two domains.

Correlation of SI with B-Factor

For every residue in the dimer protein, we calculated the average SI and associated average B-Factor. Then we normalized the B-Factor using min-max normalization and computed the correlation between the average SI and the normalized B-Factor. We found that in most cases the correlation coefficient was positive but there were a few dimers for which the correlation was low. Shown below is a scatter plot graph of SI-B-Factor correlation for dimer 1zuy.

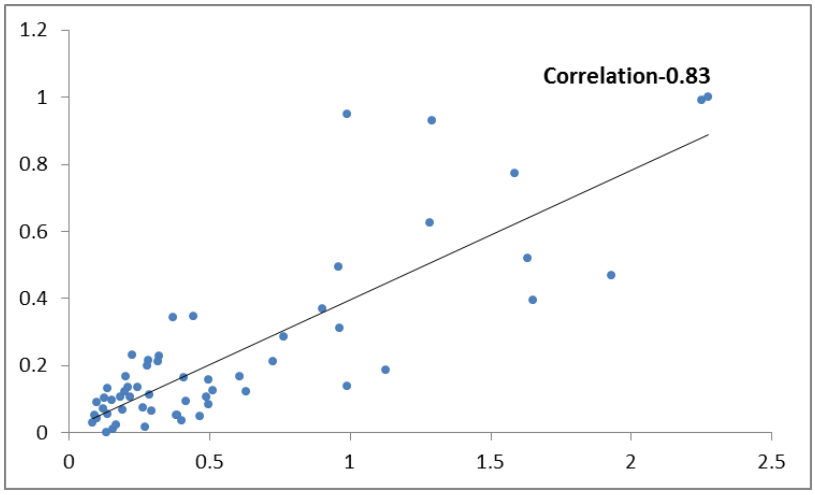

Fig. 5.8.: Dimer 1zuy with correlation 0.83

Correlation of OS with B-Factor

Similarly, for every residue in the dimer we calculated the average OS and associated average B-Factor. Then we normalized the B-Factor using the min-max normalization and computed the correlation between the average OS and the normalized B-Factor. We found that the coefficients were close to the SI-B-Factor correlation in value. Shown below is a scatter plot graph of OS-B-Factor correlation for dimer 1zuy.

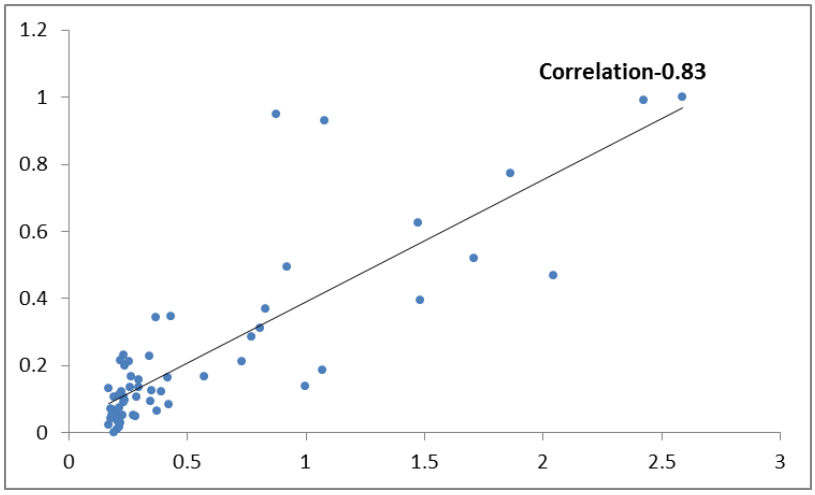

Fig. 5.9.: Dimer 1zuy with correlation 0.83

From table A.1, it can be seen that AI does not correlate that well with B-Factor from which we can infer that B-Factor does not affect AI as much.

In addition, we computed the correlation between the average OS of all residues and their associated normalized B-Factor for all the dimers together and we found the correlation to be a positive 0.36. Out of the 198 dimers, 23.7% showed a weak correlation, 39.8% showed a moderate correlation and 36.3% showed a strong correlation.

OS, SI and AI in CA and CB atoms We calculated the OS, SI and AI for the CA and CB atoms of all dimers and have listed it in table A.2. OS_CA, SI_CA, AI_CA are used as abbreviations for OS, SI and AI values for CA atoms and the same has been followed for CB atoms. From table A.2, it can be noted that the OS value for CA atoms is lesser than the CB atoms which means that CA atoms are more symmetrical as compared to CB atoms and CB atoms contribute to the off-symmetry in the dimers. We conducted a null hypothesis test to see if there was any significant difference between the mean OS for CA atoms and mean OS for CB atoms and found the p-value to be 0.04. Similarly, we conducted a null hypothesis test for mean SI and AI as well and we found the p-value to be 0.03 and 0.49 respectively.

Every residue in a chain has a CA and a CB atom. When we found that the OS_CA was lesser than the OS_CB, we computed the average B-Factor of all the CA and CB atoms in the proteins. Table A.3 shows the average B-Factor of the CA and CB atoms of each dimer. From this table we could infer that the B-Factor of CA atoms was lesser than the B-Factor of CB atoms. We conducted a hull hypothesis test to verify if there was a difference between the average B-Factors in CA and CB atoms and found the p-value to be 0.01. From this value we can conclude that there is a significant difference between the two.

5.2 Homotrimers

As already mentioned, homodimers are rotated by 120 degrees twice about the three fold axis of symmetry to calculate the off-symmetry. Shown in fig.5.10 is an example of trimer 3fuc that is rotated by 120° and 240° clockwise. It can be seen that the resultant structures are similar to the original with chains' positions changed.

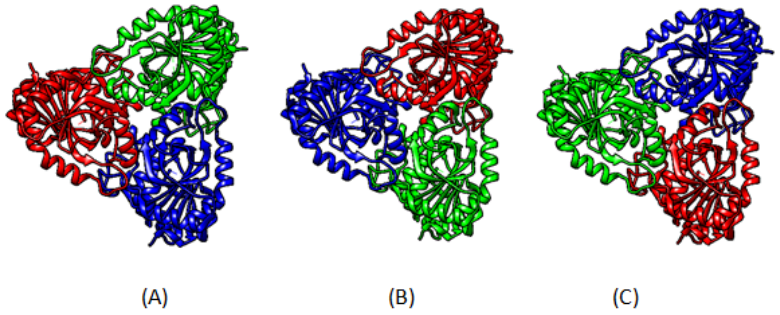

Fig. 5.10.: (A) Homotrimer 3fuc with chain A, B and C.(B) Structure (A) rotated by 120° clockwise to get C', A', B'. (C) Structure (A) rotated by 240° clockwise to get B', C', A'.

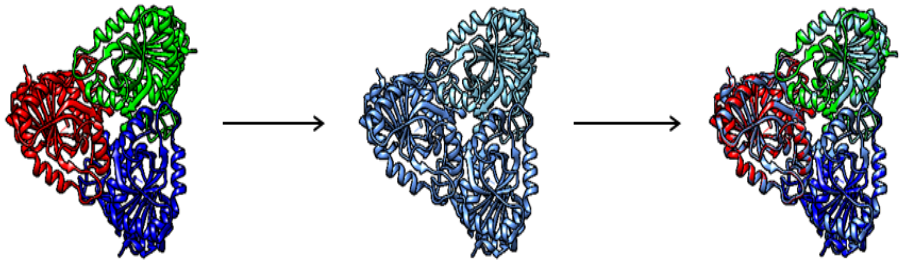

Fig. 5.11.: Structure Index in trimer 3fuc: Structural alignment of chain A and chain B produces A", chain B on chain C produces B" and chain C on chain A produces C"(middle). The difference between the newly generated A", B" and C" shown in light blue and chain B, C and A respectively in the original structure produces structure index.

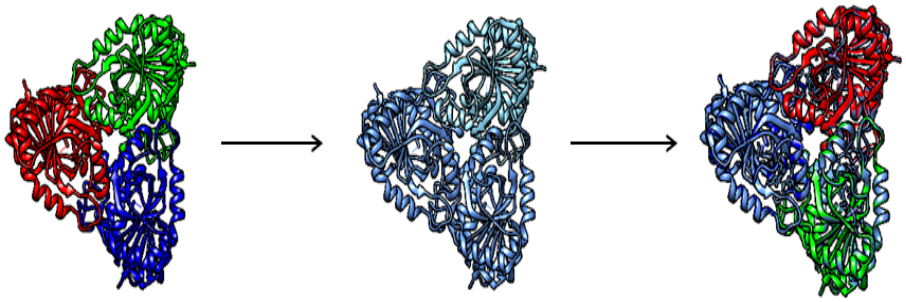

Fig. 5.12.: Assembly Index in trimer 3fuc: Structural alignment of chain A and chain B produces A", chain B on chain C produces B" and chain C on chain A produces A". The difference between the newly generated A", B" and C" shown in light blue and chain A', B' and C' produces assembly index.

The OS, SI and AI values for 58 homotrimer protein structures are listed in table A.4. Just like dimers, we found the total OS, SI, AI, average B-Factor, standard deviation of B-Factor and the B-Factor range of the trimers. The maximum and minimum values for these parameters are listed below.

Table 5.2.: Minimum and Maximum SI, AI, OS, Mean B-Factor, Stdev B-Factor and B-Factor Range in Homotrimers

Min SI	0.14
Max SI	1.49
Min AI	0.22
Max AI	2.93
Min OS	0.41
Max OS	3.04
Min Mean B-Factor	8.99
Max Mean B-Factor	31.44
Min B-FactorStdev	2.08
Max B-Factor Stdev	14.03
Min B-Factor Range	9.50
Max B-Factor Range	71.28

We calculated the correlation of SI, AI and OS with B-Factor in trimers and have listed the coefficients in table A.4. Specifically, D is the domain of the dimer, BF/OS, BF/SI and BF/AI is the correlation of OS, SI and AI with B-Factor respectively, MBF is the mean B-Factor, SBF is the standard deviation B-Factor, RBF is the B-Factor range, Å is the resolution.

Fig.5.13 shows the contribution of SI and AI to OS by comparing their mean and standard deviation (shown in the form of a vertical bar). From this figure it can be inferred that in general AI is the major contributor to OS.

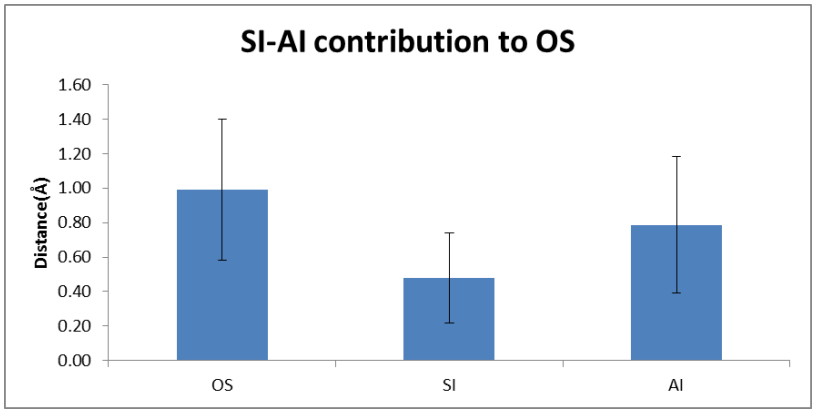

Fig. 5.13.: Contribution of AI and SI to OS in Homotrimers

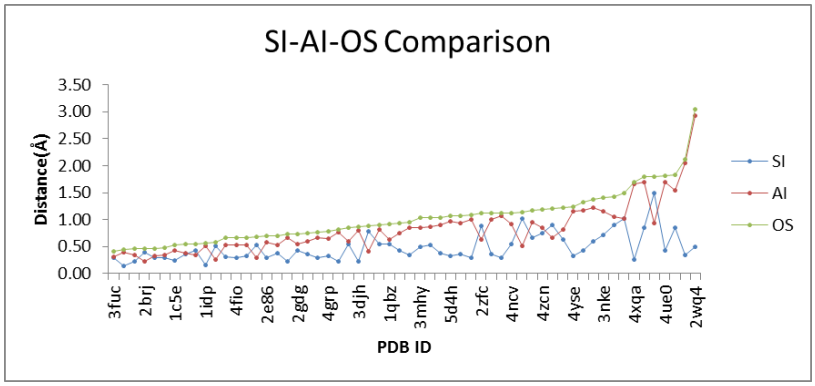

Fig. 5.14.: SI-AI-OS comparison chart for Homotrimers

In case of trimers, when the OS, SI and AI were further investigated we found that for a small OS the AI was still the major contributor while the SI was low. However, as the OS value goes higher, AI becomes almost equal to OS and can cancel out SI.

Domain-wise comparison of OS, SI and AI in trimers In table A.4, the trimers have been grouped based on their domain. Out of the 58 trimers, 36 had 1 domain and 14 had 2 domains. By calculating the average OS, SI and AI for both domains, we found out that the average values of OS, SI and AI for domain 1 was more than the average values for domain 2. Shown in fig 5.15 is a graphical representation of the comparison.

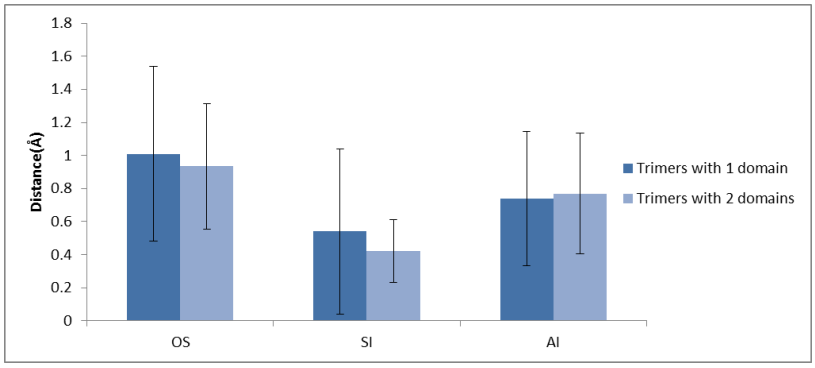

Fig. 5.15.: Domain-wise comparison of OS, SI and AI in Homotrimers

We conducted a T-test to compare the mean OS in the two domains to check if there was significant difference between the two. Using the null hypothesis, we found that the p-value was 0.409 which supports our null hypothesis.

Correlation of SI with B-Factor

For every residue in the trimer protein, we calculated the average SI and the associated average B-Factor. Then we normalized the B-Factor using min-max normalization and computed the correlation between the average SI and the normalized B-Factor. We found that the correlation coefficient was highly positive. Shown below is a scatter plot graph of SI-B-Factor correlation for trimer 4oop.

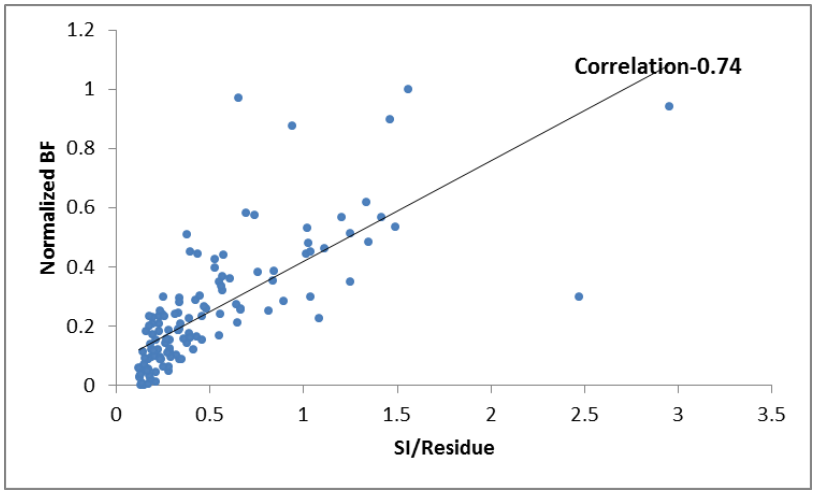

Fig. 5.16.: Trimer 4oop with correlation 0.74

Correlation of OS with B-Factor

For every residue in the trimer protein, we calculated the average OS and the associated average B-Factor. Then we normalized the B-Factor using min-max normalization and computed the correlation between the average OS and the normalized B-Factor. We found that the correlation coefficient was highly positive. Shown below is a scatter plot graph of OS-B-Factor correlation for trimer 4oop.

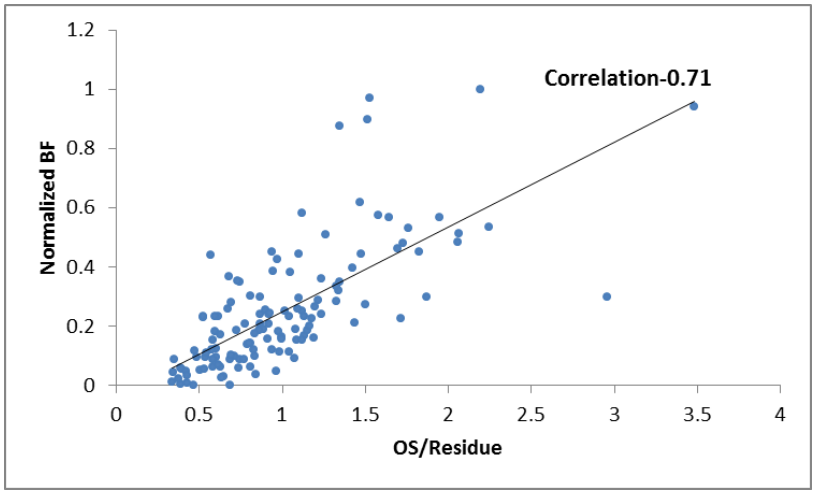

Fig. 5.17.: Trimer 4oop with correlation 0.71

It can be seen from table A.4 that AI does not have a major correlation with B-Factor but the correlation is better than in dimers. Just like in dimers, we computed the correlation between the average SI of all residues and their associated normalized B-Factor for all them together and found the correlation to be a positive 0.43. Out of the 58 trimers, 6.8% showed a weak correlation, 15.5% showed a moderate correlation and 77.58% showed a strong correlation.

OS, SI and AI in CA and CB atoms We calculated the OS, SI and AI for only the CA and CB atoms for every trimer protein. Table A.5 shows the OS, SI and AI for all the trimers. From this, it can be noted that the OS value for CA atoms is lesser than the CB atoms which means that CA atoms are more symmetrical as compared to CB atoms in trimers just as in the case of dimers. We conducted a similar null hypothesis test to see if there was a significant difference between the mean OS for CA atoms and mean OS for CB atoms and found the p-value to be 0.44 which indicates that there is no significant difference between the two averages. Similarly, we conducted a null hypothesis test for mean SI and AI as well and we found the p-value to be 0.11 and 0.3 respectively.

Similar to dimers, we computed the average B-Factor of all the CA and CB atoms in the proteins. Table A.6 shows the average B-Factor of the CA and CB atoms of each trimer. From this table we could infer that the B-Factor of CA atoms was lesser than the B-Factor of CB atoms. We conducted a null hypothesis test to verify if there was a difference between the average B-Factors in CA and CB atoms and found the p-value to be 0.06.

As the sample size for trimers is only 58, we couldn't see a high significant difference in the hypothesis test. Therefore, we decided to combine the data sets of dimers and trimers and then conducted the hypothesis test for the average B-Factor for CA and CB atoms again. We found the p-value to be 0.001. Given below is a graph that shows the comparison of average B-Factors in CA and CB atoms for dimers and trimers.

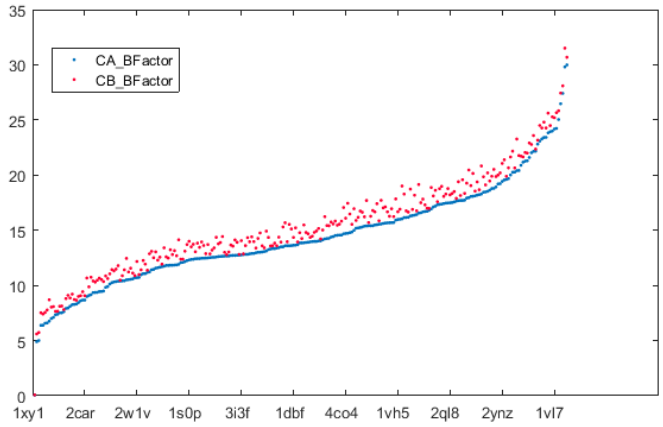

Fig. 5.18.: Comparison of average B-Factor for CA and CB atoms in dimers and trimers

As you can see, the B-Factor for CA atoms is significantly lower than the B-Factor for CB atoms.

Similarly, we combined the dimer and trimer dataset and conducted a hypothesis test to see if SI in CA atoms was significantly lower than the SI in CB atoms and found the p-value to be 0.01.

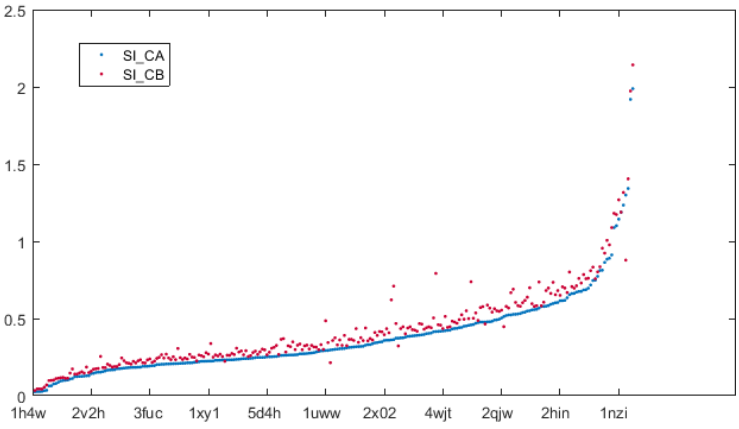

Fig. 5.19.: Comparison of SI for CA and CB atoms in dimers and trimers

By looking at both the figures, we can see that SI in CA atoms is lower than the SI in CB atoms. Also the B-Factor in CA atoms is lower than the B-Factor in CB atoms. From this we can conclude that the structure index and B-Factor are highly correlated. A high B-Factor can lead to high mobility of atoms and this contributes to the structure difference in the chains of the protein.

5.3 Rotationally unsymmetrical dimers

There are a few dimer proteins for which rotational symmetry does not work because they do not have C2 symmetry. Shown in fig 5.18 is an example of protein 2gz4 which has no paper proving that it is a homodimer.

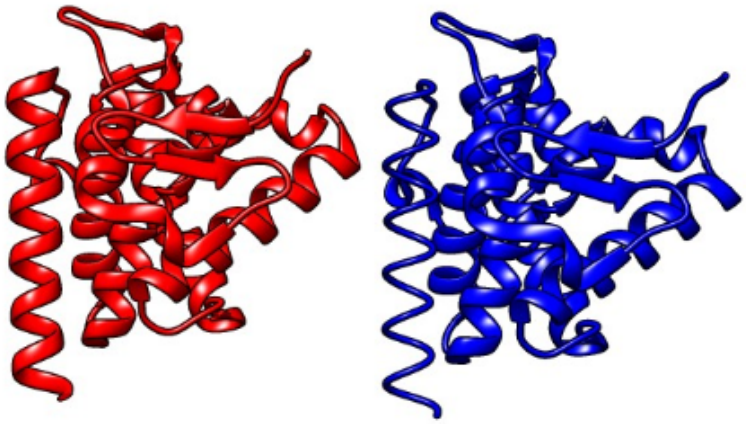

Fig. 5.20.: Rotationally unsymmetrical dimer protein- 2gz4

It can be seen that the second subunit has simply been translated and arranged similar to the first subunit, hence there is no scope for rotational symmetry. Another such protein that we discovered to having the same issue is 2gec.

5.4 Incorrectly assigned proteins

There are a few monomer proteins which have been wrongly assigned as homodimers or homotrimers in the RCSB protein data bank. The papers associated with these proteins either, do not provide any conclusive proof that these proteins are actually homodimers/homotrimers or have been described as monomers. Shown in table 5.3 and 5.4 are proteins which are actually monomers and the proteins that have no conclusive proof of being a dimer or trimer respectively.

Table 5.3.: Proteins discovered to be monomers

PDB ID	Protein Symmetry	SI	AI	OS
1o81	c1	1.11	14.50	14.38
5a71	c1	0.59	10.25	10.37
1n0q	c2	0.52	4.160	4.208
1cku	c2	0.63	3.89	3.94
2v9b	c2	0.81	2.49	2.74
1wzd	c1	0.49	24.14	23.79
1wyx	c2	0.94	2.03	2.17
3ol0	c3	0.48	2.93	3.04
3bgu	c2	0.78	3.35	3.47

Table 5.4.: Proteins with no proof of being a homodimer or homotrimer

PDB ID	Protein Symmetry	SI	AI	OS
2anx	c2	0.52	6.33	6.39
1i6w	c2	0.70	2.43	2.66
2cvi	c2	2.85	2.06	2.61

Continued on next page

Table 5.4 – continued from previous page

PDB ID	**Protein Symmetry**	**SI**	**AI**	**OS**
4grr	c3	0.33	1.36	1.43
5b8f	c3	0.55	2.66	2.8

6. CONCLUSION AND SUMMARY

Symmetry in one of the most interesting properties in proteins and in this research we explored the factors that lead to a protein not being perfectly symmetrical. We introduced two factors, called Structure Index and Assembly Index, that contribute to the Off-Symmetry in the protein.

By computing the total OS, SI and AI we found that in dimers, when the OS is low, SI is the major contributor but as the OS increases AI starts playing a major role and potentially can cancel out SI. In case of trimers, AI is the major contributor when compared to SI. Most of the proteins in our dataset, either had one domain or two domains. By comparing the average OS, SI and AI for both domains we found that there was a significant difference between the two in dimers but not in trimers.

To evaluate whether molecular dynamics can play a role in protein off-symmetry, we investigated the correlation between OS or SI or AI and B-Factor, which reflects the fluctuation of the atoms in the protein from their mean position. We calculated the OS, AI and SI values for each residue as well as B-Factor for each residue for every structure and then calculated the Pearson Coefficients. We found that in the case of both dimers and trimers, SI appears to be more correlated to the B-Factors than the other two parameters, with 90% samples having positive correlation between AI and B-Factor. Among them 11.6% has strong positive correlation and 35.4% has moderate positive correlation. These data suggest that it is possible molecular dynamics play a role in generation of protein off-symmetry. This seems to be supported by another observation of CA and CB atoms. It is known that CA atom is less mobile than CB and therefore has lower B-factor than CB, which is also confirmed by our data set. Interestingly and consistently, a lower off-symmetry is observed in CA than in CB atoms in almost all pdbs. Although B factors of the crystal structures can reflect the mobility or flexibility of various parts of the molecule in the model in general, it also

absorbs errors and can be influenced by the quality of X-ray diffraction data. This could contribute to the reason why not all samples appear to have a strong correlation between their SI and B factors residue wise.

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APPENDICES

A. TABLES

Table A.1.: OS, SI and AI correlation with B-Factor in Homodimers

PDB	D	SI	AI	OS	BF/OS	BF/SI	BF/AI	MBF	SBF	RBF	Å
1c9o	1	0.75	0.24	0.78	0.62	0.61	-0.02	16.17	5.42	24.28	1.17
1dj0	1	0.52	0.10	0.53	0.45	0.43	0.36	19.63	6.17	40.04	1.5
1djt	1	0.73	0.81	1.14	0.71	0.65	0.49	19.8	5.86	25.64	1.2
1e7l	2	0.62	0.13	0.64	0.35	0.37	0.47	26.63	6.22	36.54	1.32
1e9g	1	0.26	0.08	0.43	0.56	0.55	0.30	15.84	6.32	41.72	1.15
1eaj	1	0.42	0.17	0.45	0.18	0.15	0.33	19.79	6.48	36.43	1.35
1ezg	1	0.53	1.55	1.71	0.49	0.60	0.43	16.35	4.05	25.07	1.4
1f9z	1	1.33	0.38	1.16	0.24	0.25	0.32	21.08	9.61	54.05	1.5
1g6u	1	0.76	0.12	0.76	0.59	0.60	0.20	15.18	3.45	13.17	1.48
1gve	1	0.67	0.73	1.01	0.71	0.70	0.42	14.98	5.7	33.31	1.38
1gyo	1	1.06	0.54	1.13	0.39	0.40	0.19	20.41	8.92	50.25	1.2
1gyx	1	0.69	0.17	0.68	0.31	0.29	0.25	5.94	3.47	16.31	1.35
1h41	2	0.12	0.02	0.14	0.47	0.47	0.32	14.02	5.43	32.89	1.5
1h4w	1	0.09	0.02	0.10	0.38	0.38	-0.33	16.7	5.91	34.74	1.5
1i0r	1	1.24	0.42	1.23	0.65	0.66	0.03	24.64	10.27	51.85	1.5
1i4u	1	0.37	0.16	0.41	0.68	0.70	0.39	17.67	6.93	45.06	1.15
1ijy	1	0.99	1.47	1.92	0.47	0.41	0.36	16.09	4.97	24.97	1.35
1iq6	1	0.82	0.31	0.82	0.64	0.62	0.71	18.56	4.99	23.91	1.5
1isu	1	0.57	2.95	3.07	0.31	0.58	0.26	14.6	4.6	20.77	1.5
1ix9	2	0.38	0.59	0.78	0.39	0.50	0.13	10.59	3.74	23.87	0.9

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Table A.1 – continued from previous page

PDB	D	SI	AI	OS	BF/OS	BF/SI	BF/AI	MBF	SBF	RBF	Å
1iyb	1	1.04	0.75	1.52	0.33	0.33	0.26	11.45	4.2	23.5	1.5
1jr8	1	0.92	0.42	0.73	0.58	0.54	0.64	20.22	6.09	29.61	1.5
1k20	1	0.44	0.37	0.59	0.24	0.58	0.05	13.11	3.87	25.4	1.5
1k3y	2	0.32	0.09	0.33	0.73	0.74	0.29	20.46	8.24	59.87	1.3
1kdg	2	0.19	0.08	0.18	0.41	0.44	0.58	13.96	3.98	21.79	1.5
1kqp	1	0.36	0.22	0.48	0.62	0.61	0.34	16.33	6.05	30.4	1.03
1l6r	1	0.59	0.34	0.72	0.38	0.35	0.29	15.95	4.75	32.86	1.4
1lq9	1	0.80	0.26	0.89	0.62	0.64	-0.05	13.36	4.59	20.42	1.3
1m2d	1	0.42	0.08	0.42	0.82	0.80	0.12	16.53	7.39	32	1.05
1m4i	1	0.55	0.41	0.71	0.69	0.64	0.57	15.52	6.09	30.82	1.5
1mkk	1	0.69	0.20	0.70	0.57	0.54	0.49	21.9	7.07	33.05	1.32
1mxr	1	0.43	0.07	0.43	0.43	0.57	-0.45	19.75	6.78	38.38	1.42
1nki	1	0.36	0.58	0.75	0.74	0.75	0.16	14.5	5.6	24.22	0.95
1nww	1	0.43	1.09	1.26	0.39	0.52	-0.22	15.47	5.02	29.35	1.2
1nxm	1	0.60	0.29	0.57	0.72	0.73	0.39	8.74	3.19	17.68	1.3
1nzi	2	1.45	1.12	1.08	0.50	0.37	0.00	19.91	4.95	21.54	1.5
1o1h	1	0.14	0.05	0.15	0.67	0.68	-0.07	9.68	4.52	23.51	1.4
1ofz	1	0.36	0.85	1.11	0.36	0.63	0.06	14.3	4.21	25.52	1.5
1oi6	1	0.42	0.21	0.48	0.63	0.67	0.32	12.17	4.47	25	1.4
1oki	2	0.12	0.05	0.15	0.28	0.29	0.35	19.48	5.38	26.99	1.4
1psr	1	0.67	0.10	0.66	0.57	0.57	0.37	16.36	11.81	77.07	1.05
1pvm	2	0.86	0.48	0.86	0.47	0.47	0.51	14.42	5.42	25.54	1.5
1pyz	1	0.70	0.50	0.78	0.59	0.63	0.63	19.09	4.36	14.42	1.25
1q6o	1	0.37	0.33	0.51	0.47	0.49	0.41	15.3	3.8	17.93	1.2
1qks	2	0.33	0.37	0.34	0.67	0.64	0.35	11.32	4.01	23.88	1.28
1ql0	1	0.19	0.06	0.20	0.48	0.48	0.38	10.9	4.04	30.02	1.1

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Table A.1 – continued from previous page

PDB	D	SI	AI	OS	BF/OS	BF/SI	BF/AI	MBF	SBF	RBF	Å
1qlw	1	0.33	0.23	0.44	0.35	0.25	0.37	18.78	6.58	64.65	1.09
1rku	1	1.04	0.47	1.12	0.76	0.75	0.62	24.1	8.14	41.96	1.47
1s0p	1	0.52	0.17	0.53	0.41	0.38	0.41	14.16	5.48	25.03	1.4
1sby	1	0.46	0.09	0.46	0.69	0.68	0.14	15.87	7.15	41	1.1
1sh8	1	1.51	0.53	1.61	0.71	0.64	-0.01	15.64	7.27	33.29	1.5
1sj1	1	0.21	0.09	0.25	0.62	0.62	0.54	14.8	4.3	20.74	1.5
1sqs	1	0.66	0.30	0.73	0.55	0.51	0.59	18.17	6.59	31.29	1.5
1sr7	1	0.69	0.92	1.20	0.33	0.34	0.38	19.9	6.9	36.39	1.46
1t6f	1	1.03	0.30	1.01	0.50	0.54	0.27	15.13	3.42	15.69	1.47
1u07	1	0.80	0.53	0.98	0.47	0.47	0.11	20.63	6.34	26.68	1.13
1u0k	2	0.77	1.08	1.37	0.60	0.55	0.31	16.6	5.36	25.78	1.5
1ucr	1	1.02	0.30	1.11	0.35	0.37	0.14	17.08	8.2	32.3	1.2
1usc	1	0.40	0.14	0.41	0.65	0.65	0.41	13.89	5.6	26.96	1.24
1uwk	1	0.17	0.09	0.22	0.72	0.71	0.40	11.3	4.9	28.35	1.19
1uww	1	0.47	0.42	0.65	0.44	0.48	0.31	22.61	4.19	20.31	1.4
1uz3	1	0.94	2.41	2.74	0.04	0.32	0.04	15.13	5	28.43	1.1
1v8h	1	0.70	0.20	0.71	0.60	0.54	0.49	14.31	4.57	19.51	1.2
1v9y	1	0.50	0.08	0.52	0.53	0.52	0.28	19.39	6.4	34.11	1.32
1vh5	1	0.47	0.21	0.54	0.54	0.57	0.50	17.5	4.5	18.88	1.34
1vl7	1	0.27	0.09	0.29	0.56	0.59	0.37	34.88	5.8	32.52	1.5
1vzi	2	0.32	0.07	0.32	0.70	0.68	0.49	17.42	6.29	31.18	1.15
1w23	1	0.25	0.28	0.38	0.67	0.70	0.23	14.74	7.58	75.21	1.08
1w2i	1	0.58	0.33	0.71	0.37	0.36	0.15	14.32	2.87	11.28	1.5
1wkq	1	0.45	0.11	0.45	0.60	0.61	0.38	10.77	3.66	14.96	1.17
1wpn	1	0.32	0.10	0.35	0.70	0.71	0.54	13.36	4.4	21.47	1.3
1x2i	1	0.68	0.28	0.71	0.66	0.58	0.71	13.38	5	23.67	1.45

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Table A.1 – continued from previous page

PDB	D	SI	AI	OS	BF/OS	BF/SI	BF/AI	MBF	SBF	RBF	Å
1x9i	1	0.41	0.16	0.45	0.55	0.57	0.58	12.72	3.5	16.99	1.16
1xrk	1	0.39	0.17	0.43	0.35	0.37	0.34	13.03	3.3	17.34	1.5
1xy1	1	0.59	0.27	0.62	0.77	0.79	-0.20	0.14	0.05	0.17	1.04
1y5h	1	0.54	0.52	0.72	0.77	0.77	0.17	24.75	6.23	32.6	1.5
1yuz	2	0.36	0.12	0.37	0.56	0.60	0.12	12.89	3.38	13.45	1.4
1zrs	2	0.69	0.30	0.59	0.46	0.49	0.12	13.6	5	25.15	1.5
1zuy	1	0.59	0.24	0.58	0.84	0.83	0.56	28.02	7.99	31.29	1.39
2aib	1	0.40	0.96	1.03	0.37	0.29	0.27	14.11	2.76	14.17	1.1
2aml	2	0.23	0.15	0.26	0.36	0.39	0.15	21.11	2.89	14.55	1.5
2arc	1	0.41	0.96	1.09	0.52	0.72	0.43	19.43	7.28	35.24	1.5
2axw	1	2.24	1.17	2.71	0.51	0.58	0.42	14.48	5.7	26.71	1.05
2c5a	1	0.34	0.31	0.45	0.70	0.72	0.54	11.21	4.82	27.13	1.4
2car	1	0.46	0.09	0.47	0.69	0.70	-0.14	11.71	5.5	27.87	1.09
2d8d	1	0.68	0.13	0.68	0.63	0.62	0.17	11.28	2.9	13.04	1.15
2dkj	2	0.58	0.44	0.44	0.63	0.63	0.26	10.03	3.85	20.24	1.15
2dpf	2	0.64	0.15	0.65	0.64	0.62	0.37	22.76	6.67	41	1.5
2dpl	2	0.69	0.29	0.71	0.40	0.36	0.25	25.03	6.28	28.24	1.43
2ds5	1	0.35	0.11	0.35	0.64	0.62	0.71	14.17	4.16	14.75	1.5
2dsk	1	0.30	1.42	1.47	0.47	0.52	0.35	14.9	4.35	21.51	1.5
2dxu	2	0.60	0.30	0.67	0.71	0.69	0.30	15.33	5.45	27.12	1.28
2dy0	1	0.50	0.16	0.55	0.71	0.75	0.10	11.88	5.13	26.77	1.25
2e5f	2	0.24	0.06	0.25	0.43	0.45	-0.24	10.83	3.75	22.29	1.35
2e6f	2	0.15	0.03	0.15	0.70	0.70	0.40	8.06	2.5	17.04	1.26
2ecu	1	0.52	0.16	0.48	0.38	0.37	-0.06	9.68	3.25	14.03	1.3
2egv	1	0.92	0.07	0.91	0.74	0.75	0.21	16.06	6.14	29.48	1.45
2ehp	1	1.01	0.61	1.32	0.60	0.57	0.54	14.85	4.38	17.41	1.3

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Table A.1 – continued from previous page

PDB	D	SI	AI	OS	BF/OS	BF/SI	BF/AI	MBF	SBF	RBF	Å
2f22	1	0.67	0.16	0.72	0.51	0.49	0.48	5.58	4.06	20.85	1.42
2fnu	1	0.25	0.22	0.32	0.61	0.62	0.47	17.66	5.6	43.64	1.5
2ftr	1	0.27	0.37	0.50	0.25	0.29	0.18	19.6	2.01	8.17	1.4
2g84	1	0.43	0.12	0.45	0.68	0.67	0.40	14.08	4.8	27.54	1.4
2glz	1	0.27	0.37	0.44	0.52	0.32	0.52	31.49	7.01	39.83	1.45
2gom	1	0.74	1.03	1.41	0.46	0.56	0.37	16.28	2.8	11.81	1.25
2gty	1	0.44	0.16	0.48	0.32	0.26	0.50	17.05	2.73	10.94	1.3
2gu9	1	0.34	0.04	0.35	0.59	0.58	0.62	13.74	4.08	17.07	1.4
2gyq	1	0.94	0.28	0.97	0.42	0.38	0.55	14.77	4.9	25.88	1.4
2h8g	1	0.47	0.18	0.51	0.65	0.63	0.32	26.25	7.11	29.78	1.5
2hin	1	0.96	0.45	1.12	0.65	0.57	0.72	13.82	2.69	12.1	1.05
2i3d	1	0.24	0.07	0.25	0.49	0.49	0.55	17.52	5.9	31.45	1.5
2i51	1	0.25	0.17	0.32	0.39	0.39	0.36	19.22	4.36	19.87	1.4
2i8t	1	0.42	0.06	0.43	0.52	0.53	-0.01	9.16	2.69	11.96	1.3
2ibd	2	0.76	0.29	0.86	0.31	0.38	0.02	19.08	4.56	18.667	1.5
2ipr	1	0.78	1.35	1.66	0.64	0.63	0.63	18.45	4.7	19.52	1.5
2it2	1	1.40	0.82	1.75	0.25	0.28	-0.09	17.52	5.54	23.39	1.5
2j73	1	0.46	0.42	0.66	0.52	0.54	0.47	17.27	4.11	17.34	1.4
2jae	1	0.25	0.34	0.32	0.67	0.58	0.46	11.22	5.09	43.43	1.25
2jhf	2	0.16	0.09	0.22	0.60	0.59	0.26	13.65	3.78	36.16	1
2nlv	1	0.61	0.53	0.81	0.42	0.39	0.34	11.91	3.34	14.8	1.3
2nxv	1	0.22	0.08	0.23	0.61	0.60	0.12	12.35	4.47	29.81	1.1
2ob3	1	0.29	0.07	0.30	0.68	0.68	0.35	7.9	3.55	33.49	1.04
2odk	2	0.76	0.44	0.83	0.67	0.51	0.54	17.15	4.94	20.97	1.4
2ofc	1	0.27	0.12	0.30	0.18	0.18	0.43	8.47	3.03	14.38	1.11
2p8i	2	0.69	0.23	0.71	0.63	0.60	0.36	13.7	4.06	23.88	1.4

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Table A.1 – continued from previous page

PDB	D	SI	AI	OS	BF/OS	BF/SI	BF/AI	MBF	SBF	RBF	Å
2pa7	1	0.55	0.17	0.60	0.67	0.65	0.27	24.53	7.82	40.56	1.5
2peb	1	0.29	0.32	0.46	0.66	0.72	0.23	28.9	6.17	32.9	1.46
2phn	1	0.35	0.07	0.37	0.38	0.37	-0.16	18.61	6.53	30.04	1.35
2pl7	1	0.33	0.04	0.33	0.50	0.49	0.39	8.61	5.58	31.79	1
2prv	1	0.86	0.73	1.14	0.47	0.54	0.15	15.94	4.14	24.3	1.3
2prx	1	0.43	0.33	0.56	0.50	0.54	0.07	15.14	3.9	21.62	1.5
2q20	1	0.63	0.55	0.92	0.28	0.36	0.49	16.02	3.28	16.46	1.3
2q9o	3	0.10	0.10	0.12	0.49	0.48	0.37	11.48	3.98	21.16	1.3
2qe8	1	0.20	0.15	0.26	0.33	0.30	0.44	16.09	5.13	35.69	1.35
2qif	1	0.56	0.92	1.13	0.14	0.34	0.01	13.79	5.9	27.53	1.5
2qjw	2	0.62	0.37	0.69	0.48	0.48	0.43	15.18	3.83	19.35	1.35
2ql8	1	0.29	0.31	0.46	0.45	0.35	0.34	18.68	4.83	24.58	1.5
2r5o	1	1.35	0.28	1.38	0.26	0.27	0.05	17.06	3.5	19.6	1.3
2r8q	1	0.27	0.32	0.41	0.63	0.63	0.41	22.59	6.81	47.96	1.5
2rc8	2	0.41	0.07	0.41	0.43	0.44	0.28	11.72	6.02	34.68	1.45
2rl8	1	0.79	0.24	0.78	0.61	0.58	0.36	16.21	5.17	25.79	1.45
2v27	1	0.61	0.40	0.86	0.72	0.71	0.25	14.4	6.7	43.22	1.5
2vha	1	0.26	0.36	0.49	0.45	0.62	0.25	12.32	6.61	31.99	1
2voc	1	0.42	0.29	0.54	0.47	0.51	0.10	14.86	4.21	19.38	1.5
2vok	1	0.34	0.77	0.88	0.60	0.71	0.48	18.27	4.27	20.43	1.3
2vv6	2	0.77	0.69	0.98	0.61	0.66	0.22	23.04	4.27	15.01	1.5
2w1v	1	0.13	0.03	0.13	0.50	0.50	0.43	11.34	3.23	23.81	1.49
2w2a	1	0.08	0.02	0.08	0.56	0.56	0.35	10.83	3.19	16.28	1.38
2w31	1	0.67	0.13	0.69	0.57	0.56	0.49	18.25	5.71	29.52	1.5
2w3g	1	0.91	2.52	2.67	0.39	0.60	0.44	21.05	6.51	27.96	1.4
2w3p	2	0.20	0.05	0.22	0.58	0.57	0.25	14.89	4.05	21.8	1.5

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Table A.1 – continued from previous page

PDB	D	SI	AI	OS	BF/OS	BF/SI	BF/AI	MBF	SBF	RBF	Å
2w6a	1	2.51	0.91	2.47	0.43	0.32	0.40	14.15	3.91	22.1	1.4
2wtp	1	0.89	0.14	0.89	0.65	0.64	0.53	18.04	8.14	35.67	1.5
2wu9	1	0.54	0.14	0.45	0.53	0.54	0.31	11.34	6.94	36.99	1.5
2wuj	1	1.14	0.29	1.18	0.16	0.09	-0.10	21.27	9.8	42.06	1.4
2x02	1	0.49	0.61	0.86	0.36	0.32	0.69	17.22	6.24	27.37	1.35
2xhf	1	0.61	0.33	0.74	0.58	0.59	0.06	23.9	10.77	59.43	1.3
2xi8	1	0.71	0.42	0.82	0.18	0.17	0.12	17.2	4.7	19.64	1.21
2xmj	1	0.34	0.22	0.40	0.64	0.60	0.55	7.74	2.38	10.09	1.08
2y53	1	0.24	0.05	0.21	0.63	0.64	0.46	10.11	5.17	39.3	1.4
2yna	1	0.57	0.26	0.61	0.49	0.45	0.41	21.03	8.53	40.3	1.5
2yve	1	0.96	0.78	1.25	0.38	0.50	0.31	15.92	5.03	23.08	1.4
2z6r	2	0.92	0.31	0.95	0.58	0.56	0.21	18.69	5.47	26.34	1.5
2zcm	1	1.38	0.49	1.45	0.27	0.20	-0.03	18.21	4.84	22.63	1.33
2zdp	1	0.39	0.11	0.39	0.61	0.57	0.24	14.82	5.21	21.55	1.5
2zew	1	0.72	1.56	1.79	0.18	0.25	0.54	19.02	4.3	21.95	1.4
2zvx	1	0.55	0.99	1.24	0.49	0.64	-0.03	14.54	4.34	20.72	1.09
3a6r	2	0.40	0.10	0.42	0.56	0.58	0.21	14.54	2.74	12.2	1.2
3aia	1	0.41	0.06	0.41	0.68	0.68	0.65	20.82	5.98	26.37	1.4
3ayj	2	0.30	0.04	0.27	0.60	0.59	0.47	14.09	5.25	32.76	1.1
3b0f	1	0.82	0.24	0.84	0.12	0.11	0.17	9.47	2.74	13.26	1.4
3b4u	1	0.31	0.05	0.31	0.62	0.63	-0.11	11.16	3.71	17.8	1.2
3bje	1	0.30	0.06	0.31	0.57	0.55	0.35	20.68	6.13	35.78	1.44
3bmz	1	0.38	0.12	0.42	0.54	0.56	0.50	14.75	4.01	18.37	1.21
3bxu	1	0.74	1.90	2.06	0.48	0.65	0.32	8.04	2.71	11.75	1.35
3c3y	1	0.44	0.22	0.50	0.62	0.60	0.31	16.95	5.08	25.76	1.37
3c8e	1	0.70	0.34	0.63	0.66	0.62	0.41	13.34	4.61	25.65	1.5

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Table A.1 – continued from previous page

PDB	D	SI	AI	OS	BF/OS	BF/SI	BF/AI	MBF	SBF	RBF	Å
3c9u	2	0.53	0.20	0.60	0.44	0.39	0.79	22.5	8.09	46.43	1.48
3ccd	1	0.16	0.02	0.17	0.53	0.54	0.00	7.94	2.31	12.34	1
3cov	1	0.73	0.14	0.72	0.55	0.53	0.13	17.47	6.92	37.16	1.5
3cp7	2	0.59	0.09	0.63	0.32	0.32	0.47	12.34	3.56	16.61	1.39
3ct6	1	0.65	0.07	0.65	0.57	0.56	0.63	17.12	8.15	45.5	1.1
3ctp	2	0.23	0.06	0.24	0.60	0.61	0.55	15.52	6.8	36.98	1.41
3cwr	1	0.46	0.39	0.65	0.49	0.38	0.63	23.22	6.17	19.48	1.5
3f1l	1	0.50	0.29	0.53	0.16	0.53	0.13	16.12	11.51	62.16	0.95
3g46	1	0.50	0.48	0.71	0.52	0.57	0.37	12.79	3.22	16.79	0.91
3vrc	1	0.62	0.82	1.15	0.34	0.27	-0.08	14.68	6.88	37.44	1
4axo	1	0.71	0.15	0.76	0.32	0.35	0.68	13.74	4.92	19.35	1
4nds	1	0.36	0.25	0.43	0.46	0.45	-0.23	8.86	2.9	12.17	1
4nsv	1	0.11	0.08	0.16	0.59	0.62	0.22	8.3	2.95	19.42	0.9
4qiu	1	0.40	0.27	0.53	0.56	0.57	0.24	16.87	5.02	25.93	1.4
4rt5	1	0.74	0.37	0.57	0.52	0.32	-0.54	20.99	9.35	52.25	1.5
4unu	1	0.57	1.24	1.33	0.53	0.57	0.34	7.82	3.2	25.2	0.95
4wjt	1	0.51	0.32	0.37	0.60	0.53	0.18	20.88	8.83	43.92	1.21
4yag	1	0.12	0.03	0.16	0.54	0.54	0.46	19.28	7.34	35.54	1.5
4ypo	1	0.84	0.29	1.08	0.46	0.42	0.25	17.46	6.07	35.15	1
4ysl	1	0.36	0.12	0.28	0.36	0.43	0.49	26.03	7.01	37.68	1.46
5i5m	1	0.14	0.07	0.14	0.58	0.61	0.33	8.83	3.5	22.5	1.37
5idb	1	0.46	0.56	0.76	0.52	0.51	0.16	8.7	3.28	18.12	1

Table A.2.: OS, SI, AI values of CA and CB atoms in Homodimers

PDB ID	**OS_CA**	**SI_CA**	**AI_CA**	**OS_CB**	**SI_CB**	**AI_CB**
1c9o	0.44200	0.40615	0.20683	0.47438	0.44021	0.18464
1dj0	0.40984	0.39416	0.10133	0.47183	0.46356	0.09942
1djt	0.81383	0.37494	0.76268	0.84367	0.44612	0.73702
1e7l	0.43919	0.42415	0.12522	0.46616	0.44688	0.13518
1e9g	0.24011	0.23222	0.07065	0.27044	0.26118	0.07887
1eaj	0.34469	0.30639	0.16812	0.42279	0.39058	0.18593
1ezg	1.62034	0.30069	1.58218	1.66685	0.37477	1.63249
1f9z	0.94209	1.29944	0.72373	0.88527	0.87800	0.38922
1g6u	0.49162	0.50321	0.11382	0.55528	0.55430	0.16175
1gve	0.80914	0.55557	0.58500	0.84248	0.59561	0.58558
1gyo	0.82663	0.74607	0.56433	0.96879	0.83269	0.47750
1gyx	0.48103	0.54830	0.27715	0.64356	0.63780	0.29757
1h41	0.10319	0.09849	0.01913	0.12232	0.11822	0.02213
1h4w	0.02834	0.02572	0.01378	0.03574	0.03374	0.01336
1i0r	0.81281	0.91180	0.49052	1.05987	1.08843	0.52790
1i4u	0.24700	0.21314	0.12409	0.27849	0.25028	0.11868
1ijy	1.68191	0.61772	1.47446	1.70768	0.69725	1.42910
1iq6	0.62088	0.68674	0.38201	0.77601	0.75762	0.40092
1isu	3.18083	0.32730	3.14347	2.99747	0.43857	3.06799
1ix9	0.55306	0.27301	0.42409	0.60027	0.32749	0.44291
1iyb	1.28622	0.88998	0.89947	1.44794	0.97712	0.91220
1jr8	0.36682	0.77337	0.66594	0.64972	0.80188	0.66838
1k20	0.43386	0.27541	2.88934	0.46227	0.30269	0.10826
1k3y	0.20077	0.18365	0.08549	0.22452	0.21254	0.09590

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Table A.2 – continued from previous page

PDB ID	OS_CA	SI_CA	AI_CA	OS_CB	SI_CB	AI_CB
1kdg	0.18601	0.16851	0.07848	0.20471	0.18874	0.08038
1kqp	0.39120	0.31407	0.22018	0.43229	0.36497	0.22238
1l6r	0.52129	0.38725	0.33276	0.55902	0.42781	0.34208
1lq9	0.68047	0.57994	0.26212	0.76889	0.68080	0.25021
1m2d	0.21276	0.20671	0.08186	0.24012	0.23358	0.08820
1m4i	0.52870	0.34395	0.40389	0.56555	0.39046	0.39166
1mkk	0.44674	0.44200	0.20183	0.52388	0.52393	0.20209
1mxr	0.39769	0.39094	0.10722	0.42560	0.41752	0.10826
1nki	0.61573	0.20542	0.57160	0.74394	0.26877	0.65333
1nww	1.21525	0.38899	1.08486	1.24074	0.42460	1.09192
1nxm	0.42697	0.45860	0.28532	0.48274	0.73773	0.28639
1nzi	0.87537	1.18886	1.07598	0.93361	1.18886	0.96312
1o1h	0.12958	0.12251	0.04303	0.14780	0.13981	0.04643
1ofz	1.06864	0.29663	3.28817	1.07123	0.21394	3.24198
1oi6	0.33819	0.27668	0.20033	0.38667	0.32594	0.21496
1oki	0.03286	0.02812	0.01638	0.04773	0.04316	0.01983
1psr	0.46475	0.47376	0.13071	0.48630	0.48755	0.10519
1pvm	0.75492	0.74833	0.53904	0.79003	0.75734	0.52801
1pyz	0.45846	0.12880	0.45015	0.48905	0.18566	0.48463
1q6o	0.38052	0.29290	0.27275	0.52275	0.48533	0.37079
1qks	0.47542	0.30486	0.37003	0.48995	0.32614	0.37232
1ql0	0.15050	0.14295	0.05540	0.16500	0.15877	0.05046
1qlw	0.24562	0.24227	0.08170	0.26697	0.25981	0.07596
1rku	0.95290	0.86320	0.46017	0.99283	0.92335	0.44192
1s0p	0.35817	0.34905	0.17741	0.41831	0.41387	0.17878
1sby	0.33395	0.33066	0.08622	0.37423	0.37004	0.08361

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Table A.2 – continued from previous page

PDB ID	OS_CA	SI_CA	AI_CA	OS_CB	SI_CB	AI_CB
1sh8	1.29272	1.23410	1.10123	1.40802	1.31624	1.06646
1sj1	0.08294	0.06356	0.05371	0.11115	0.09811	0.05567
1sqs	0.45111	0.38557	0.29549	0.51261	0.44613	0.31706
1sr7	0.87261	0.47689	0.74653	1.12548	0.57667	0.77126
1t6f	0.54244	0.52317	0.21727	0.67568	0.66715	0.29243
1u07	0.77893	0.54110	0.50651	0.81928	0.61683	0.50782
1u0k	1.22883	0.59202	1.05608	1.28965	0.66251	1.07890
1ucr	0.89664	0.81259	0.29802	1.05068	0.95497	0.38692
1usc	0.26325	0.25767	0.11601	0.27401	0.26709	0.10483
1uwk	0.16772	0.14968	0.09855	0.19194	0.17416	0.09216
1uww	0.50030	0.29332	0.41651	0.53439	0.34425	0.41654
1uz3	2.22716	0.58347	2.09478	2.52456	0.69701	2.02505
1v8h	0.45105	0.43598	0.16704	0.47326	0.46920	0.15684
1v9y	0.19226	0.18341	0.05027	0.22933	0.22270	0.06206
1vh5	0.20717	0.17707	0.10094	0.48138	0.24407	0.11264
1vl7	0.20842	0.18501	0.07534	0.24576	0.22594	0.06944
1vzi	0.21107	0.20140	0.07140	0.24704	0.24167	0.07236
1w23	0.34072	0.20921	0.27456	0.37511	0.24600	0.27632
1w2i	0.42839	0.27911	0.33278	0.46826	0.31592	0.35333
1wkq	0.27250	0.26614	0.10457	0.32704	0.32695	0.13532
1wpn	0.21191	0.18056	0.09860	0.24133	0.21275	0.10576
1x2i	0.41684	0.37948	0.26564	0.43536	0.40122	0.21478
1x9i	0.23033	0.21079	0.10846	0.30037	0.24416	0.10475
1xrk	0.28093	0.25452	0.11840	0.35772	0.32578	0.11365
1xy1	0.30369	0.22437	0.18446	0.38553	0.33774	0.25857
1y5h	0.64915	0.53848	0.44243	0.74759	0.60254	0.50270

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Table A.2 – continued from previous page

PDB ID	OS_CA	SI_CA	AI_CA	OS_CB	SI_CB	AI_CB
1yuz	0.25625	0.23987	0.10140	0.28152	0.26508	0.09163
1zrs	0.29104	0.52273	0.42067	0.46980	0.56822	0.45935
1zuy	0.40530	0.41922	0.25536	0.44512	0.43505	0.17275
2aib	0.99535	0.31731	0.96312	1.08066	0.43431	1.07136
2aml	0.26322	0.21048	0.13961	0.28625	0.23450	0.14687
2arc	0.67238	0.31588	0.60084	1.23044	0.35786	0.62900
2axw	2.42273	1.91909	1.13085	2.42470	1.97309	1.13303
2c5a	0.44551	0.33690	0.31113	0.47212	0.36038	0.31709
2car	0.15134	0.15276	0.05777	0.25577	0.25448	0.06340
2d8d	0.39806	0.39666	0.12227	0.42777	0.43033	0.11478
2dkj	0.67676	0.55736	0.45528	0.69788	0.57858	0.44966
2dpf	0.36073	0.35818	0.15500	0.40656	0.39514	0.15058
2dpl	0.48532	0.45551	0.28063	0.53653	0.49914	0.25859
2ds5	0.23531	0.23153	0.10762	0.22707	0.22262	0.08484
2dsk	1.42655	0.21769	1.41734	1.45137	0.22583	1.44052
2dxu	0.50823	0.42398	0.29128	0.52504	0.44279	0.29476
2dy0	0.38515	0.33063	0.15993	0.41037	0.35546	0.16114
2e5f	0.13399	0.12734	0.04117	0.15309	0.14653	0.03916
2e6f	0.09920	0.10145	0.02868	0.11426	0.11369	0.02499
2ecu	0.29361	0.34760	0.16783	0.37109	0.41583	0.19028
2egv	0.65263	0.67089	0.07459	0.69949	0.71222	0.07988
2ehp	0.64723	0.88377	0.71184	0.97285	1.00588	0.84065
2f22	0.53690	0.49546	0.16239	0.59411	0.54579	0.18855
2fnu	0.30216	0.21632	0.20942	0.32807	0.24767	0.21560
2ftr	0.25106	0.24117	0.07008	0.27178	0.25368	0.10856
2g84	0.28321	0.26399	0.11370	0.33165	0.31788	0.09838

Continued on next page

Table A.2 – continued from previous page

PDB ID	OS_CA	SI_CA	AI_CA	OS_CB	SI_CB	AI_CB
2glz	0.26236	0.20807	0.18810	0.46464	0.23388	0.19048
2gom	0.69880	0.37248	0.57242	0.80311	0.46747	0.62558
2gty	0.32491	0.29104	0.12424	0.33495	0.30014	0.13358
2gu9	0.08080	0.07964	0.01155	0.23456	0.11077	0.01379
2gyq	0.64511	0.66196	0.30436	0.71171	0.70646	0.25737
2h8g	0.33954	0.28995	0.17208	0.37322	0.33044	0.15977
2hin	0.80306	0.61549	0.44167	0.84955	0.70490	0.48713
2i3d	0.11940	0.10818	0.06016	0.15730	0.14661	0.06300
2i51	0.24343	0.17515	0.16268	0.26690	0.20207	0.16379
2i8t	0.24611	0.24060	0.05134	0.29097	0.29128	0.06809
2ibd	0.55071	0.51943	0.19680	0.60690	0.57820	0.17416
2ipr	1.51332	0.55962	1.32445	1.56073	0.58275	1.33017
2it2	1.45030	1.08864	0.80605	1.53151	1.18125	0.79149
2j73	0.47148	0.26416	0.41007	0.53537	0.34883	0.41493
2jae	0.39663	0.22511	0.32651	0.42043	0.24954	0.33896
2jhf	0.17203	0.12564	0.08067	0.17826	0.15505	0.09019
2nlv	0.65319	0.45008	0.44502	0.68263	0.49520	0.42454
2nxv	0.15014	0.17509	0.05439	0.17522	0.18915	0.05669
2ob3	0.19234	0.18271	0.06614	0.21314	0.20460	0.07530
2odk	0.60421	0.47667	0.39683	0.67410	0.57065	0.37281
2ofc	0.20086	0.16601	0.11433	0.22803	0.20438	0.09930
2p8i	0.52452	0.49132	0.22499	0.57677	0.55001	0.22086
2pa7	0.45615	0.40344	0.16937	0.54572	0.44647	0.19650
2peb	0.28480	0.20368	0.18326	0.33233	0.26522	0.17700
2phn	0.20143	0.19486	0.03265	0.22986	0.22377	0.03842
2pl7	0.21150	0.20828	0.03127	0.31182	0.30624	0.05774

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Table A.2 – continued from previous page

PDB ID	OS_CA	SI_CA	AI_CA	OS_CB	SI_CB	AI_CB
2prv	0.76318	0.56677	0.67183	0.90314	0.73622	0.71721
2prx	0.40184	0.26098	0.31120	0.48337	0.36506	0.33449
2q20	0.67904	0.39229	0.52822	0.76227	0.46702	0.57190
2q9o	0.09490	0.07627	0.05379	0.14035	0.10135	0.05646
2qe8	0.15749	0.16070	0.08732	0.17887	0.18168	0.09142
2qif	0.92585	0.29795	0.86779	0.97316	0.35737	0.89982
2qjw	0.51724	0.51245	0.20664	0.47118	0.44702	0.14854
2ql8	0.37099	0.23208	0.28380	0.46516	0.26243	0.28151
2r5o	1.15627	1.14333	0.25012	1.33038	1.26843	0.22631
2r8q	0.41951	0.25207	0.31996	0.42758	0.26582	0.32228
2rc8	0.28650	0.31237	0.10142	0.36192	0.36472	0.10103
2rl8	0.52781	0.57801	0.32440	0.60047	0.58194	0.28955
2v27	0.74548	0.47715	0.39743	0.76295	0.46466	0.47481
2vha	1.43234	0.15240	1.42174	0.35032	0.17613	1.45338
2vk8	0.34716	0.26320	0.03830	0.40251	0.32320	0.25019
2voc	0.34716	0.24889	0.21740	0.85179	0.29682	0.78556
2vok	0.73962	0.47887	0.68027	0.85390	0.56695	0.67017
2vv6	0.03496	0.03518	0.00604	0.06729	0.06987	0.01970
2w1v	0.02986	0.02659	0.01204	0.04535	0.04394	0.01499
2w2a	0.02987	0.02659	0.01205	0.04534	0.04392	0.01329
2w31	0.42023	0.41526	0.11908	0.53947	0.79213	0.25792
2w3p	0.17654	0.16674	0.04893	0.20558	0.19578	0.04815
2w6a	2.14655	1.98819	0.88583	2.19266	2.14229	0.73630
2wtp	0.47105	0.47852	0.08933	0.56987	0.58710	0.15758
2wu9	0.40275	0.48199	0.25771	0.54237	0.54139	0.27152
2wuj	0.68880	0.65376	0.24132	0.85071	0.80107	0.28304

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Table A.2 – continued from previous page

PDB ID	OS_CA	SI_CA	AI_CA	OS_CB	SI_CB	AI_CB
2x02	0.65944	0.35917	0.48249	0.70652	0.43370	0.48586
2xhf	0.41955	0.24767	0.31577	0.44202	0.28391	0.31610
2xi8	0.64834	0.54995	0.35442	0.78731	0.69904	0.35899
2xmj	0.25510	0.19076	0.18712	0.28530	0.23165	0.17572
2y53	0.21347	0.20572	0.03941	0.25295	0.24464	0.04716
2yna	0.47645	0.44106	0.26728	0.53795	0.49276	0.30034
2yve	1.00372	0.69594	0.75738	1.06074	0.76045	0.77221
2z6r	0.72299	0.68496	0.29013	0.80956	0.78458	0.31357
2zcm	1.15053	1.10069	0.63594	1.24580	1.17317	0.64381
2zdp	0.21993	0.22381	0.10268	0.27291	0.27861	0.10335
2zew	1.68111	0.60349	1.50272	1.73640	0.68052	1.51833
2zvx	0.73874	0.26199	0.68083	0.83814	0.36969	0.69690
3a6r	0.20998	0.18539	0.09107	0.25246	0.23304	0.07599
3aia	0.24383	0.23879	0.06286	0.29696	0.28996	0.06417
3ayj	0.26929	0.26472	0.06935	0.30646	0.29890	0.07151
3b0f	0.48816	0.46927	0.21399	0.55021	0.53583	0.22301
3b4u	0.19650	0.18986	0.04769	0.22047	0.21365	0.05048
3bje	0.18888	0.19034	0.05547	0.21011	0.21182	0.05640
3bmz	0.26340	0.23600	0.09280	0.30646	0.28301	0.08697
3bxu	1.93793	0.52693	1.85096	2.03411	0.68954	1.86117
3c3y	0.35960	0.28647	0.21121	0.37255	0.29802	0.23000
3c8e	0.44124	0.63437	0.48962	0.58664	0.66828	0.51053
3c9u	0.25597	0.23247	0.08192	0.29558	0.27362	0.08429
3ccd	0.03768	0.03296	0.01792	0.05787	0.05513	0.01774
3cov	0.59771	0.60230	0.14881	0.64612	0.65397	0.16738
3cp7	0.44731	0.45141	0.12742	0.53845	0.55004	0.19256

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Table A.2 – continued from previous page

PDB ID	OS_CA	SI_CA	AI_CA	OS_CB	SI_CB	AI_CB
3ct6	0.31179	0.32022	0.05075	0.35208	0.35691	0.06390
3ctp	0.11890	0.11166	0.05405	0.17264	0.17346	0.06416
3cwr	0.57869	0.38414	0.35561	0.62104	0.43807	0.34200
3f1l	0.41170	0.36318	0.31322	4.24449	0.70971	0.31915
3g46	0.46446	0.36157	0.29944	0.62516	0.62057	0.50400
3vrc	0.85384	0.48961	0.63666	0.90361	0.56337	0.62540
4axo	0.42658	0.41402	0.11023	0.52467	0.50411	0.12958
4nds	0.32398	0.23534	0.24812	0.38288	0.30758	0.24331
4nsv	0.12600	0.09975	0.07739	0.13782	0.11228	0.08015
4qiu	0.38568	0.24764	0.26581	0.39868	0.26804	0.25805
4rt5	0.31044	0.52758	0.38079	0.39184	0.60410	0.42519
4unu	0.95566	0.41776	1.15244	0.96558	0.45647	1.13635
4wjt	0.26886	0.42070	0.31459	0.31828	0.51313	0.38188
4yag	0.10093	0.09553	0.03189	0.12987	0.11609	0.04088
4ypo	0.86646	0.81088	0.44228	0.94667	0.83502	0.44281
4ysl	0.09371	0.28330	0.23962	0.25026	0.31447	0.26301
5i5m	0.13155	0.12407	0.06004	0.14891	0.14053	0.06809
5idb	0.51153	0.27206	0.42721	0.54344	0.32279	0.42518

Table A.3.: Comparison of average B-Factor in CA and CB atoms in Homodimers

PDB ID	CA B-Factor	CB B-Factor
1c9o	13.12	14.92
1dj0	17.92	19.27
1djt	16.30	18.73

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Table A.3 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
1e7l	23.83	25.62
1e9g	11.56	13.04
1eaj	16.93	18.88
1ezg	14.52	15.83
1f9z	16.15	18.28
1g6u	12.62	13.89
1gve	13.97	14.46
1gyo	18.08	20.15
1gyx	5.00	5.73
1h41	12.96	13.39
1h4w	15.21	16.17
1i0r	23.94	24.49
1i4u	14.99	16.95
1ijy	14.56	15.55
1iq6	17.46	18.28
1isu	11.83	13.23
1ix9	9.36	10.30
1iyb	10.13	11.05
1jr8	18.63	19.46
1k20	11.81	12.59
1k3y	17.68	19.40
1kdg	13.03	13.59
1kqp	12.47	13.62
1l6r	14.84	15.54
1lq9	11.42	13.09
1m2d	13.59	15.68

Continued on next page

Table A.3 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
1m4i	14.13	15.02
1mkk	19.43	21.06
1mxr	18.07	19.05
1nki	12.76	14.06
1nww	13.99	14.81
1nxm	7.51	8.11
1nzi	18.45	19.85
1o1h	8.25	9.21
1ofz	13.30	13.58
1oi6	10.42	11.41
1oki	17.48	18.78
1psr	13.24	14.35
1pvm	12.72	13.56
1pyz	15.68	16.27
1q6o	13.99	14.93
1qks	10.59	11.12
1ql0	9.82	10.86
1qlw	17.35	18.77
1rku	22.81	23.17
1s0p	12.35	13.50
1sby	13.61	15.12
1sh8	13.91	14.68
1sj1	13.64	14.35
1sqs	16.58	17.50
1sr7	17.57	18.51
1t6f	13.60	13.96

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Table A.3 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
1u07	16.56	19.15
1u0k	15.41	15.70
1ucr	14.22	16.23
1usc	11.85	13.15
1uwk	9.44	10.66
1uww	21.17	21.65
1uz3	12.64	14.43
1v8h	12.43	13.83
1v9y	15.56	17.71
1vh5	16.00	16.91
1vl7	24.23	25.66
1vzi	14.78	16.47
1w23	12.72	14.12
1w2i	13.34	13.60
1wkq	9.35	10.40
1wpn	11.81	12.48
1x2i	11.65	12.56
1x9i	12.09	12.38
1xrk	12.07	12.38
1xy1	0.06	0.07
1y5h	24.18	25.20
1yuz	12.67	12.79
1zrs	12.48	12.88
1zuy	26.47	27.44
2aib	12.90	14.40
2aml	20.27	20.65

Continued on next page

Table A.3 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
2arc	17.11	18.11
2axw	11.74	13.41
2c5a	9.90	10.62
2car	8.99	10.67
2d8d	9.37	10.47
2dkj	9.09	9.87
2dpf	20.42	21.77
2dpl	23.42	24.27
2ds5	12.54	13.20
2dsk	12.74	13.91
2dxu	13.85	14.78
2dy0	10.35	11.48
2e5f	9.49	10.35
2e6f	7.62	7.81
2ecu	8.11	8.86
2egv	13.60	15.53
2ehp	13.42	14.37
2f22	4.90	5.60
2fnu	15.67	16.67
2ftr	18.47	19.11
2g84	12.82	13.61
2glz	29.99	30.68
2gom	15.55	15.86
2gty	15.41	16.27
2gu9	12.16	13.10
2gyq	13.34	13.83

Continued on next page

Table A.3 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
2h8g	25.04	25.83
2hin	12.42	13.05
2i3d	16.42	16.76
2i51	17.19	18.62
2i8t	8.60	9.07
2ibd	18.12	18.55
2ipr	17.31	17.59
2it2	21.60	22.91
2j73	15.70	16.24
2jae	10.70	10.89
2jhf	12.55	13.40
2nlv	10.56	11.56
2nxv	11.07	11.93
2ob3	6.39	7.40
2odk	15.19	15.89
2ofc	7.52	8.13
2p8i	11.83	12.80
2pa7	22.15	23.59
2peb	27.41	28.09
2phn	17.70	18.15
2pl7	6.76	8.70
2prv	14.03	15.16
2prx	12.90	13.97
2q20	14.42	15.57
2q9o	10.52	11.22
2qe8	14.25	15.43

Continued on next page

Table A.3 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
2qif	10.51	12.45
2qjw	13.89	14.80
2ql8	17.51	18.33
2r5o	16.17	16.65
2r8q	20.89	21.72
2rc8	10.25	11.43
2rl8	14.27	15.41
2v27	13.07	13.41
2vha	10.38	11.79
2voc	13.85	14.25
2vok	17.63	17.89
2vv6	22.17	22.36
2w1v	10.73	10.98
2w2a	10.39	10.48
2w31	16.70	17.30
2w3g	19.68	20.66
2w3p	14.04	14.22
2w6a	11.86	12.69
2wtp	14.68	17.06
2wu9	9.45	10.53
2wuj	18.92	19.87
2x02	15.69	16.95
2xhf	18.28	20.83
2xi8	15.50	17.41
2xmj	6.38	7.52
2y53	8.67	9.43

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Table A.3 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
2yna	17.70	19.58
2yve	14.55	15.46
2z6r	17.49	18.21
2zcm	15.62	17.03
2zdp	13.69	13.94
2zew	18.23	18.67
2zvx	12.57	14.36
3a6r	8.44	9.00
3aia	19.61	19.89
3ayj	12.71	13.66
3b0f	8.67	9.07
3b4u	10.41	10.88
3bje	19.20	20.00
3bmz	13.95	14.35
3bxu	7.34	7.65
3c3y	15.98	16.68
3c8e	12.52	12.86
3c9u	21.30	21.99
3ccd	7.39	7.66
3cov	15.48	16.67
3cp7	11.70	11.93
3ct6	11.91	14.14
3ctp	12.86	13.96
3cwr	22.03	22.78
3f1l	12.31	14.00
3g46	11.45	12.51

Continued on next page

Table A.3 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
3vrc	12.82	14.33
4axo	11.06	12.26
4nds	7.00	8.03
4nsv	6.57	7.55
4qiu	15.37	16.22
4rt5	17.37	18.98
4unu	6.60	7.77
4wjt	17.95	20.46
4yag	15.41	16.79
4ypo	13.86	15.48
4ysl	23.41	24.80
5i5m	8.31	8.66
5idb	7.10	8.08

Table A.4.: OS, SI and AI correlation with B-Factor in Homotrimers

PDB	D	SI	AI	OS	BF/OS	BF/SI	BF/AI	MBF	SBF	RBF	Å
1c5e	1	0.24	0.43	0.53	0.60	0.88	0.14	14.78	6.08	43.37	1.1
1dbf	1	0.42	0.34	0.55	0.47	0.37	0.42	16.40	6.36	31.40	1.3
1gd0	1	0.22	0.66	0.73	0.67	0.60	0.44	16.58	3.85	19.61	1.5
1idp	1	0.15	0.51	0.57	0.71	0.67	0.52	18.81	8.89	52.55	1.45
1jlj	1	0.14	0.40	0.45	0.61	0.61	0.22	20.54	7.11	48.22	1.6
1pwb	2	0.59	1.23	1.38	0.81	0.74	0.59	17.45	7.36	40.17	1.4
1qbz	1	0.54	0.64	0.92	0.57	0.68	0.45	20.66	8.21	40.38	1.47
1sg4	1	0.66	0.96	1.16	0.71	0.69	0.44	22.81	7.92	40.58	1.3

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Table A.4 – continued from previous page

PDB	D	SI	AI	OS	BF/OS	BF/SI	BF/AI	MBF	SBF	RBF	Å
1sjm	2	0.29	0.34	0.48	0.69	0.67	0.62	13.66	4.18	21.50	1.4
1snr	2	0.31	0.53	0.66	0.71	0.71	0.25	14.49	4.09	20.62	1.31
1uxa	1	0.42	0.75	0.93	0.73	0.67	0.75	21.32	7.35	35.34	1.5
1vmf	1	0.35	2.05	2.12	0.64	0.67	0.53	20.42	3.69	20.17	1.46
1wrv	2	0.30	0.32	0.47	0.62	0.61	0.3	12.74	4.38	25.94	1.5
2bcm	1	0.42	1.17	1.32	0.62	0.59	0.4	22.48	3.60	17.80	1.48
2brj	1	0.40	0.22	0.46	0.60	0.57	0.49	11.73	4.45	20.26	1.5
2e86	2	0.30	0.58	0.70	0.71	0.68	0.45	13.09	3.82	17.24	1.5
2gdg	1	0.42	0.55	0.74	0.65	0.71	0.13	19.49	5.55	28.32	1.45
2j9c	1	0.90	0.67	1.20	0.77	0.75	-0.03	18.40	7.11	30.59	1.3
2pp8	2	0.32	0.53	0.66	0.67	0.62	0.44	17.42	4.89	23.77	1.5
2v2h	1	0.23	0.35	0.46	0.43	0.54	0.04	12.90	7.14	46.51	1.18
2wpz		1.01	1.02	1.49	0.64	0.65	0.27	17.83	4.80	18.60	1.25
2wq4	1	3.04	0.49	2.93	0.63	0.81	0.69	9.26	4.38	21.03	1.42
2yny	1	1.49	0.94	1.79	0.39	0.50	0.06	18.87	8.28	40.21	1.35
2ynz	1	0.79	0.42	0.88	0.19	0.28	0.15	21.55	10.38	43.69	1.4
2zfc	1	0.88	0.63	1.11	0.45	0.28	0.76	24.87	8.13	38.59	1.5
3djh	1	0.23	0.79	0.87	0.70	0.38	0.67	13.34	2.08	9.50	1.25
3fuc	1	0.29	0.30	0.41	0.75	0.66	0.74	17.67	6.22	26.67	1.45
3h0u	1	0.36	0.37	0.54	0.67	0.56	0.54	13.91	3.68	18.18	1.5
3i3f	1	0.35	0.84	0.95	0.20	0.49	-0.06	13.02	2.64	9.89	1.35
3ijj	1	0.22	0.76	0.81	0.69	0.56	0.67	13.70	3.34	19.99	1.25
3mhy	1	0.50	0.85	1.03	0.60	0.64	0.46	18.00	4.79	22.79	1.4
3ncq	1	0.51	0.26	0.59	0.83	0.84	0.35	22.13	11.56	51.82	1.24
3ncr	1	0.53	0.29	0.67	0.85	0.86	0.63	25.48	14.03	71.28	1.44
3nke	1	0.71	1.16	1.41	0.58	0.62	0.45	17.63	4.45	23.37	1.4

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Table A.4 – continued from previous page

PDB	D	SI	AI	OS	BF/OS	BF/SI	BF/AI	MBF	SBF	RBF	Å
3qxz	2	0.38	0.90	1.04	0.64	0.61	0.62	11.84	4.22	21.87	1.35
3rwn	2	0.29	0.66	0.76	0.68	0.68	0.46	9.68	2.20	11.18	1
4b0h	1	0.84	1.69	1.79	0.56	0.50	0.44	11.23	5.15	26.80	1.18
4co4	1	0.54	0.59	0.84	0.64	0.58	0.37	17.99	5.93	31.14	1.5
4fio	2	0.30	0.53	0.66	0.35	0.51	0.09	16.55	6.31	35.01	1.37
4fn7	1	0.38	0.54	0.71	0.64	0.67	0.44	13.89	5.64	34.72	1.25
4grn	1	0.37	1.00	1.11	0.69	0.58	0.53	14.14	3.82	26.34	1.25
4grp	1	0.33	0.65	0.78	0.71	0.75	0.31	13.62	4.83	27.62	1.27
4gvq	2	0.63	0.81	1.22	0.62	0.51	0.58	14.51	5.57	38.58	1.3
4k6v	1	0.30	1.07	1.12	0.87	0.57	0.87	24.15	7.02	36.01	1.5
4k6w	1	0.29	1.00	1.08	0.52	0.62	0.1	25.01	7.38	35.89	1.5
4ncv	1	0.54	0.91	1.12	0.84	0.67	0.75	14.82	4.32	19.16	1.2
4oop	2	0.53	0.87	1.03	0.71	0.74	0.75	18.34	5.16	25.08	1.5
4rfu		0.37	0.59	0.74	0.49	0.43	0.38	13.85	7.02	40.21	1.2
4ue0		0.43	1.69	1.81	0.69	0.68	0.47	18.42	7.61	33.83	1.17
4usi	1	0.84	1.54	1.84	0.74	0.66	0.3	19.21	7.35	32.17	1.45
4xqa	2	0.25	1.66	1.70	0.73	0.52	0.16	31.44	6.90	34.10	1.41
4yse	3	0.32	1.15	1.23	0.78	0.78	0.59	16.20	5.80	36.95	1.2
4zcn		0.74	0.85	1.19	0.71	0.67	0.44	8.99	3.21	15.59	1.3
5a95	2	0.54	0.81	0.90	0.73	0.70	0.34	11.91	5.31	43.76	1.35
5apu		1.02	0.51	1.14	0.62	0.63	0.29	22.71	7.37	34.99	1.35
5b4o	1	0.36	0.94	1.08	0.71	0.63	0.5	17.36	4.14	18.62	1.37
5d4h	3	0.33	0.97	1.07	0.62	0.63	0.44	17.10	6.10	36.45	1.3
5jbx	2	0.91	1.05	1.43	0.45	0.46	0.54	14.76	4.55	24.65	1.1

Table A.5.: OS, SI, AI values of CA and CB atoms in Homotrimers

PDB ID	OS_CA	SI_CA	AI_CA	OS_CB	SI_CB	AI_CB
1c5e	0.46347	0.17867	0.42410	0.50391	0.22646	0.41989
1dbf	0.38403	0.22990	0.33796	0.39966	0.26908	0.33863
1gd0	0.67660	0.13000	0.65977	0.67853	0.14949	0.65605
1idp	0.51312	0.06441	0.51407	0.52838	0.09932	0.51454
1jlj	0.41081	0.08756	0.39187	0.42671	0.11358	0.39200
1pwb	1.26052	0.43544	1.21661	1.29479	0.47647	1.25077
1qbz	0.71866	0.30436	0.63994	0.73833	0.36095	0.61010
1sg4	1.04968	0.53189	0.95006	1.09844	0.57908	0.97172
1sjm	0.40413	0.21258	0.34480	0.42361	0.23797	0.34910
1snr	0.59201	0.22309	0.53459	0.60943	0.25265	0.53680
1uxa	0.81570	0.27135	0.75357	0.85648	0.33505	0.75705
1vmf	2.05636	0.19258	2.05684	2.07130	0.23820	2.05251
1wrv	0.37036	0.18173	0.32402	0.38643	0.21024	0.31823
2bcm	1.18074	0.22411	1.16186	1.19044	0.26945	1.15726
2brj	0.31970	0.24797	0.22082	0.36744	0.30190	0.22656
2e86	0.64020	0.22928	0.58350	0.65692	0.25741	0.58854
2gdg	0.60291	0.26227	0.54801	0.62128	0.28291	0.55124
2j9c	0.93464	0.57817	0.66682	0.96402	0.60524	0.68767
2pp8	0.59240	0.23376	0.53152	0.61169	0.26669	0.53602
2v2h	0.38864	0.14532	0.34870	0.40701	0.17166	0.35345
2wpz	1.05009	0.46084	0.98043	1.10709	0.50142	1.00456
2wq4	2.99759	0.37249	2.93617	3.02562	0.32238	2.94537
2yny	1.65326	1.34180	0.91955	1.67848	1.40446	0.86954
2ynz	0.72838	0.61502	0.42045	0.75106	0.65030	0.41038

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Table A.5 – continued from previous page

PDB ID	OS_CA	SI_CA	AI_CA	OS_CB	SI_CB	AI_CB
2zfc	0.69763	0.41657	0.59586	0.74135	0.45981	0.60988
3djh	0.81220	0.12531	0.79903	0.81816	0.14755	0.80087
3fuc	0.32550	0.19421	0.29928	0.34267	0.21559	0.30332
3h0u	0.50159	0.30989	0.37537	0.51555	0.32389	0.38122
3i3f	0.89026	0.24700	0.84721	0.90918	0.28852	0.84847
3ijj	0.78770	0.15617	0.76917	0.79733	0.18213	0.77532
3mhy	0.92503	0.35922	0.85093	0.97506	0.40727	0.86963
3ncq	0.36552	0.27151	0.26143	0.39805	0.29757	0.24333
3ncr	0.47515	0.31904	0.28599	0.52564	0.37557	0.32337
3nke	1.29491	0.52947	1.15854	1.31571	0.58341	1.14100
3qxz	0.99453	0.31830	0.90048	1.02153	0.34600	0.92459
3rwn	0.71965	0.20701	0.67363	0.73625	0.25244	0.65917
4b0h	1.74822	0.67576	1.69313	1.78321	0.72983	1.69420
4co4	0.74616	0.40225	0.60068	0.78723	0.44007	0.61658
4fio	0.55830	0.16773	0.52951	0.56747	0.18568	0.51821
4fn7	0.59492	0.24333	0.53894	0.61822	0.27941	0.53569
4grn	1.02065	0.22303	0.99933	1.04599	0.25933	1.01512
4grp	0.68037	0.20228	0.64511	0.69204	0.24866	0.65053
4gvq	1.06162	0.43272	0.79860	1.09901	0.48250	0.79804
4k6v	1.03725	0.25233	0.99467	1.06820	0.30759	1.00616
4k6w	0.78744	0.22007	0.74848	0.80830	0.26354	0.75691
4ncv	0.95739	0.34226	0.89564	1.00332	0.40925	0.90765
4oop	0.90982	0.37419	0.86208	0.94127	0.43451	0.84713
4rfu	0.69668	0.30213	0.59524	0.70811	0.32917	0.59258
4ue0	1.68732	0.25337	1.67410	1.70781	0.31304	1.65495
4usi	1.74577	0.66273	1.53286	1.78234	0.69651	1.54640

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Table A.5 – continued from previous page

PDB ID	OS_CA	SI_CA	AI_CA	OS_CB	SI_CB	AI_CB
4xqa	1.69615	0.21284	1.67001	1.73568	0.26773	1.67967
4yse	1.17566	0.22925	1.15472	1.20189	0.26416	1.17396
4zcn	1.06138	0.59676	0.83227	1.17254	0.73435	0.83938
5a95	0.81962	0.23152	0.77369	0.82267	0.25335	0.76511
5apu	1.14337	0.67505	1.02323	1.15435	0.75912	1.04345
5b4o	0.96516	0.20398	0.93182	0.98564	0.24357	0.94292
5d4h	1.01793	0.25231	0.97077	1.03585	0.28167	0.97772
5jbx	1.30544	0.71719	1.19377	1.38406	0.80978	1.22130

Table A.6.: Comparison of average B-Factor in CA and CB atoms in Homotrimers

PDB ID	CA B-Factor	CB B-Factor
1c5e	13.01	14.76
1dbf	13.65	15.22
1gd0	14.56	15.82
1idp	17.42	18.07
1jlj	18.19	19.38
1pwb	16.33	16.89
1qbz	18.53	20.2
1sg4	20.26	22.17
1sjm	12.67	13.03
1snr	13.5	13.93
1uxa	18.8	20.52
1vmf	18.78	19.89
1wrv	11.6	12.29

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Table A.6 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
2bcm	21.26	22.05
2brj	11.17	11.38
2e86	12.75	12.81
2gdg	16.37	18.18
2j9c	15.65	17.12
2pp8	16.81	16.98
2v2h	10.7	12.17
2wpz	13.5	15.3
2wq4	8.28	8.72
2yny	15.39	17.7
2ynz	19.56	21.39
2zfc	20.4	23.27
3djh	12.65	13
3fuc	16.72	17
3h0u	13.39	13.6
3i3f	12.8	12.86
3ijj	12.37	13.73
3mhy	16.03	19.01
3ncq	19.22	20.2
3ncr	23.28	24.27
3nke	16.16	16.76
3qxz	10.97	11.41
3rwn	7.91	8.81
4b0h	9.16	10.74
4co4	14.73	17.45
4fio	14.71	16.09

Continued on next page

Table A.6 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
4fn7	13	14.26
4grn	12.25	13.71
4grp	11.22	12.87
4gvq	12.46	13.94
4k6v	23.09	24.5
4k6w	23.99	25.28
4ncv	12.61	13.77
4oop	16.66	17.82
4rfu	12.49	13.71
4ue0	15.92	17.84
4usi	17.73	18.34
4xqa	29.81	31.51
4yse	14.38	15.75
4zcn	7.95	9.1
5a95	10.31	11.32
5apu	20.01	21.64
5b4o	15.3	16.63
5d4h	15.25	16.74
5jbx	12.43	13.45
1usc	11.85	13.15
1uwk	9.44	10.66
1uww	21.17	21.65
1uz3	12.64	14.43
1v8h	12.43	13.83
1v9y	15.56	17.71
1vh5	16	16.91

Continued on next page

Table A.6 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
1vl7	24.23	25.66
1vzi	14.78	16.47
1w23	12.72	14.12
1w2i	13.34	13.6
1wkq	9.35	10.4
1wpn	11.81	12.48
1x2i	11.65	12.56
1x9i	12.09	12.38
1xrk	12.07	12.38
1xy1	0.06	0.07
1y5h	24.18	25.2
1yuz	12.67	12.79
1zrs	12.48	12.88
1zuy	26.47	27.44
2aib	12.9	14.4
2aml	20.27	20.65
2arc	17.11	18.11
2axw	11.74	13.41
2c5a	9.9	10.62
2car	8.99	10.67
2d8d	9.37	10.47
2dkj	9.09	9.87
2dpf	20.42	21.77
2dpl	23.42	24.27
2ds5	12.54	13.2
2dsk	12.74	13.91

Continued on next page

Table A.6 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
2dxu	13.85	14.78
2dy0	10.35	11.48
2e5f	9.49	10.35
2e6f	7.62	7.81
2ecu	8.11	8.86
2egv	13.6	15.53
2ehp	13.42	14.37
2f22	4.9	5.6
2fnu	15.67	16.67
2ftr	18.47	19.11
2g84	12.82	13.61
2glz	29.99	30.68
2gom	15.55	15.86
2gty	15.41	16.27
2gu9	12.16	13.1
2gyq	13.34	13.83
2h8g	25.04	25.83
2hin	12.42	13.05
2i3d	16.42	16.76
2i51	17.19	18.62
2i8t	8.6	9.07
2ibd	18.12	18.55
2ipr	17.31	17.59
2it2	21.6	22.91
2j73	15.7	16.24
2jae	10.7	10.89

Continued on next page

Table A.6 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
2jhf	12.55	13.4
2nlv	10.56	11.56
2nxv	11.07	11.93
2ob3	6.39	7.4
2odk	15.19	15.89
2ofc	7.52	8.13
2p8i	11.83	12.8
2pa7	22.15	23.59
2peb	27.41	28.09
2phn	17.7	18.15
2pl7	6.76	8.7
2prv	14.03	15.16
2prx	12.9	13.97
2q20	14.42	15.57
2q9o	10.52	11.22
2qe8	14.25	15.43
2qif	10.51	12.45
2qjw	13.89	14.8
2ql8	17.51	18.33
2r5o	16.17	16.65
2r8q	20.89	21.72
2rc8	10.25	11.43
2rl8	14.27	15.41
2v27	13.07	13.41
2vha	10.38	11.79
2voc	13.85	14.25

Continued on next page

Table A.6 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
2vok	17.63	17.89
2vv6	22.17	22.36
2w1v	10.73	10.98
2w2a	10.39	10.48
2w31	16.7	17.3
2w3g	19.68	20.66
2w3p	14.04	14.22
2w6a	11.86	12.69
2wtp	14.68	17.06
2wu9	9.45	10.53
2wuj	18.92	19.87
2x02	15.69	16.95
2xhf	18.28	20.83
2xi8	15.5	17.41
2xmj	6.38	7.52
2y53	8.67	9.43
2yna	17.7	19.58
2yve	14.55	15.46
2z6r	17.49	18.21
2zcm	15.62	17.03
2zdp	13.69	13.94
2zew	18.23	18.67
2zvx	12.57	14.36
3a6r	8.44	9
3aia	19.61	19.89
3ayj	12.71	13.66

Continued on next page

Table A.6 – continued from previous page

PDB ID	CA B-Factor	CB B-Factor
3b0f	8.67	9.07
3b4u	10.41	10.88
3bje	19.2	20
3bmz	13.95	14.35
3bxu	7.34	7.65
3c3y	15.98	16.68
3c8e	12.52	12.86
3c9u	21.3	21.99
3ccd	7.39	7.66
3cov	15.48	16.67
3cp7	11.7	11.93
3ct6	11.91	14.14
3ctp	12.86	13.96
3cwr	22.03	22.78
3f1l	12.31	14
3g46	11.45	12.51
3vrc	12.82	14.33
4axo	11.06	12.26
4nds	7	8.03
4nsv	6.57	7.55
4qiu	15.37	16.22
4rt5	17.37	18.98
4unu	6.6	7.77
4wjt	17.95	20.46
4yag	15.41	16.79
4ypo	13.86	15.48

Continued on next page

Table A.6 – continued from previous page

PDB ID	**CA B-Factor**	**CB B-Factor**
4ysl	23.41	24.8
5i5m	8.31	8.66
5idb	7.1	8.08