



Analysis of interactions between secondary structures in globular proteins
by Robert Barton Burris

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Biochemistry

Montana State University

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Abstract:

In an attempt to develop a system to aid protein structure prediction and the design of de novo proteins, residue-residue interactions in globular proteins are analyzed. Computer programs were written which studied interactions between charged atoms, polar side-chain atoms, polar backbone atoms, total backbone atoms and hydrophobic side-chain atoms. The data from these studies are analyzed and improvements in programs and new avenues of investigation are suggested.

Programs were written which would evaluate the data from the above programs. These programs have been designed to analyze the data from several perspectives. Interactions between residues were studied for the entire protein, between secondary structures in general, and between the following combinations of secondary structure pairs: 1) α -helix - α -helix, 2) α -helix - β -sheet, 3) β -sheet - α -helix, 4) β -sheet - β -sheet. For interactions between hydrophobic side chain atoms, the data were analyzed further. Interactions between pairs of residues were studied according to the angles at which the secondary structures crossed. The number of occurrences of each amino acid at each position relative to the nearest backbone contact are presented for all angle ranges. Additionally, the number of residue-residue contacts and average number of atom contacts are given for each amino acid at each position. To demonstrate the capabilities of the system to analyze data, Ala was studied for interactions between pairs of α -helices with crossing angles of -150° to -180° . For Ala at each position relative to nearest backbone atom contact, all atoms which interacted with Ala were listed according to their relative position to the nearest backbone atom contact, the number of residue-residue interactions the residue made with Ala, and the average number of atom contacts made between the two residues.

The results of the above analyses were evaluated for the heat stable protein thermolysin. The analysis of this thermophilic protein was undertaken in an attempt to provide insight into protein stability with the ultimate goal of assisting in the design of novel proteins. It is suggested that triads of α -helices, all of which interact with each other, contribute to the stability of thermolysin.

ANALYSIS OF INTERACTIONS BETWEEN SECONDARY
STRUCTURES IN GLOBULAR PROTEINS

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This thesis has been read by each member of the thesis committee and has been found to be satisfactory regarding content, English usage, format, citations, bibliographic style, and consistency, and is ready for submission to the College of Graduate Studies.

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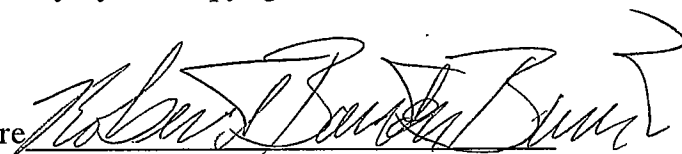
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ABSTRACT

In an attempt to develop a system to aid protein structure prediction and the design of de novo proteins, residue-residue interactions in globular proteins are analyzed. Computer programs were written which studied interactions between charged atoms, polar side-chain atoms, polar backbone atoms, total backbone atoms and hydrophobic side-chain atoms. The data from these studies are analyzed and improvements in programs and new avenues of investigation are suggested.

Programs were written which would evaluate the data from the above programs. These programs have been designed to analyze the data from several perspectives. Interactions between residues were studied for the entire protein, between secondary structures in general, and between the following combinations of secondary structure pairs: 1) α -helix - α -helix, 2) α -helix - β -sheet, 3) β -sheet - α -helix, 4) β -sheet - β -sheet. For interactions between hydrophobic side chain atoms, the data were analyzed further. Interactions between pairs of residues were studied according to the angles at which the secondary structures crossed. The number of occurrences of each amino acid at each position relative to the nearest backbone contact are presented for all angle ranges. Additionally, the number of residue-residue contacts and average number of atom contacts are given for each amino acid at each position. To demonstrate the capabilities of the system to analyze data, Ala was studied for interactions between pairs of α -helices with crossing angles of -150° to -180° . For Ala at each position relative to nearest backbone atom contact, all atoms which interacted with Ala were listed according to their relative position to the nearest backbone atom contact, the number of residue-residue interactions the residue made with Ala, and the average number of atom contacts made between the two residues.

The results of the above analyses were evaluated for the heat stable protein thermolysin. The analysis of this thermophilic protein was undertaken in an attempt to provide insight into protein stability with the ultimate goal of assisting in the design of novel proteins. It is suggested that triads of α -helices, all of which interact with each other, contribute to the stability of thermolysin.

INTRODUCTION

Protein Folding

Since Anfinsen's seminal work with the renaturation of ribonuclease, it has been widely believed that the primary sequence of a protein is sufficient to determine protein structure. The prediction of protein tertiary structure remains elusive. The advent of protein X-ray crystallography has accelerated insight into factors affecting protein structure.

Energy of Folding

The folded shape of a protein is a complex interplay between enthalpy and entropy as the protein assumes a low energy conformation. In spite of daunting efforts to predict the native state of a protein from energy calculations, there has been little success. This arises in large part from the difficulty in assigning correct enthalpic and entropic contributions to the free energy of the system. Computational time required to accurately assign energy terms to all variables appears to be prohibitive. This has necessitated that alternative avenues of investigating protein structure and stability be investigated. A major effort in this area is being assigned to pattern recognition, under the premise that rather than attempting the calculation of energy ab initio, an understanding of favorable

interactions may be more accurately ascertained through investigation of known protein structures.

The folding of a protein is widely believed to be a thermodynamic process involving the interplay between the aqueous solvent and regions of proteins which vary in hydrophobicity. While the effects of water on protein structure are not studied explicitly in this work, it is recognized that water is central in the determination of protein structure.

When hydrophobic groups are introduced into water, enthalpic and entropic changes occur. The creation of a hole in the hydrogen-bonded water structure is enthalpically unfavorable(3). However, there are favorable enthalpic contributions due to London forces between the non-polar group and water. It has been determined that the attractive force between nonpolar molecules and water is comparable to that between non-polar molecules(3). The result is that the net enthalpy of interaction of a hydrophobic group with water may be favorable.

When nonpolar groups are introduced into water, a cage of hydrogen bonded water molecules is formed. This causes the entropy of the system to decrease. Hydrophobic groups tend to self-associate in water to decrease their total solvent accessible surface area and minimize the unfavorable decrease in entropy(3). This is the basis of the dogma that hydrophobic side chains bury in the protein interior while charged and polar side-chains tend to reside on the protein surface. The amount of buried area has been related to stability(12) and the amount of solvent exposed surface can be predicted(24). Through computer

simulations, it has been shown that helices and sheets form upon polymer compaction(9) and the amount of secondary structure increases as the chain becomes increasingly compact(44).

Water affects conformations of side chains on the protein surface and is often found in active sites, where it is usually involved in mediating electrostatic strain in enzymatic activity. Water is often ordered in X-ray protein structures and is often found to interact with secondary structures where they protrude from the hydrophobic interior(2). The groups interacting with bound water tend to be charged and the affect of water at the ends of secondary structures is likely to affect the conformations of turns.

Charged Groups

The potentially charged groups in proteins are the N- and C-termini, and side chain atoms from Asp, Glu, Cys, Tyr, Lys, Arg, and His. Of these side chains, only Asp, Glu, Lys and Arg are normally charged. At physiological pH, less than one in ten His residues will carry a positive charge. This is supported by a study of potential salt-bridges where it was determined that salt-bridges involving His marginally contributed to stability(60).

The strength of interactions between ion pairs decreases with $1/r$, where r is the distance separating the centers of the atoms in question. The dependence of the dielectric constant upon groups surrounding charged atoms makes accurate prediction of the strength of charged interactions difficult. This difficulty is exacerbated when shielding effects of salt groups are taken into account. These

factors adversely affect the accuracy of models which extrapolate the cost of burying charged groups from water to non-polar solvents to the cost of burying amino acids in folded proteins. Perhaps more telling is the topological distribution of charged groups on the protein surface. An average of only one pair of interacting charged groups per 150 residues are found to be buried in the hydrophobic interior(28). When charged groups are found in the protein interior, they are usually located within 4 Å of an oppositely charged group and if not, they are nearly always hydrogen bonded to a polar group(20).

Much of the insight into contributions of charged groups on protein stability has been garnered through site-directed mutagenesis experiments and analysis of X-ray structures. Currently, charged interactions are not considered to be dominant in the determination of the folded state(9). From a statistical point of view, this is exemplified by the poor evolutionary conservation of charged groups, with the noted exception of charged groups located in binding sites and active sites(28). However, ion pairs in thermophilic proteins are often the predominant difference between these proteins and their mesophilic counterparts(45,62). There is near consensus agreement that charged groups do affect protein stability.

The position of charged groups seems to be important in determining whether they contribute to stabilization or destabilization. Intra-helical salt bridges are often formed between side chains of oppositely charged residues separated by either three or four residues(60). This was demonstrated when two peptides were synthesized, one composed of repeating blocks of glu₄ and lys₄ and the other

composed of repeating blocks of glu_2 and lys_2 (41). The peptide which repeated after four residues was stable while the peptide which repeated after two residues was not stable. The authors concluded that ion pairing was responsible for the differences in stability. While these interactions are considered to stabilize helix formation, the magnitude of the contribution to protein stability is subject to debate. The insertion of glutamate and lysine residues four residues apart on a surface helix of barnase has been estimated to contribute only 0.2 kcal/mol to stability(38). This contribution is at the lower end of salt-bridge stabilization, where estimates usually range from three to five kcal/mol. Addition of charges which cannot be well solvated and do not form intramolecular salt-bridges result in the destabilization of proteins(54,55). Clustering of positively charged groups in both bovine pancreatic trypsin inhibitor and phage T4 lysozyme result in destabilization(14,53,57). The distance over which charged groups mediate their effect is large. In subtilisin, charged groups up to 20 Å from a His residue affect the pK of that His residue(4).

Charged groups are often found at the ends of helices. There is a tendency for negatively charged groups to be found at the amino-termini of helices and for positively charged groups to be found at the carboxy-termini. This may be a result of the evolutionary drive to stabilize the helical dipole, which carries $+0.25 e^-$ at the amino end and $-0.25 e^-$ at the carboxyl end. As with nearly all other calculations of stability, there is dispute as to the magnitude of stabilization. It has been suggested, from work done on the four-helix bundle protein myohemerythrin, that interactions between charged groups and the helical dipole have been

overestimated, at least with respect to the stability of myohemerythrin(56). However, in this study, the effect of charged interactions between groups on different helices was not taken into account. Likewise, the stable de novo protein designed by DeGrado and co-workers, based upon the four-helix bundle proteins myohemerythrin, cytochrome c', and tobacco mosaic coat protein(43), analyzed the placement of charged groups solely from the standpoint of stabilization of the helical dipole. However, the antiparallel sense of helices in these models places the positively charged amino acids at the C-terminus of one helix in close proximity with negatively charged amino acids at the N-terminus of an adjacent helix. There is a paucity of information regarding the study of charged groups between the ends of different secondary structures.

A study of the preponderance of hydrogen bonds in protein structures(59) found that 80% of Asp side-chains and 72% of Glu side-chains formed hydrogen bonds through both carboxylate oxygens. For Arg side-chains, 33% had all three guanido nitrogen groups involved in hydrogen bonds, 35% had two groups hydrogen bonded, and 25% had only one group involved in hydrogen bonds. Of the hydrogen bonded guanido nitrogens, there was a preference for the terminal NH_2 groups to be involved rather than the ϵ -NH group. For Lys, 24% formed no hydrogen bonds, 36% formed one hydrogen bond, 19% formed two hydrogen bonds, 14% formed three hydrogen bonds, and 7% formed more than three hydrogen bonds, presumably through shared hydrogen bonds. Glu and especially Asp were characterized by making a high number of contacts with backbone

nitrogen atoms. Interestingly, Lys residing on the surface made fewer contacts with water than all of the other charged groups as well as Thr, Asn, Gln, and His.

The Hydrophobic Interior

The interior of a protein is dominated by hydrophobic amino acids. These amino acids utilize their wide range of dihedral angles to form low energy(7,25,32,57) close-packing structures. While some regions pack more closely than others, the overall packing density for proteins is comparable to the packing density of small organic molecules(5,22). There are very few empty regions the size of a methyl group within the protein interior(8,17).

The importance of hydrophobic packing is evidenced by the high evolutionary conservation of hydrophobic residues(58). There does not appear to exist a preference for the degree of burial of different hydrophobic groups. Large hydrophobic groups were not found to be buried more frequently or more fully than small hydrophobic groups(18). Specifics of hydrophobic interactions will be addressed more fully in the Introduction section dealing with packing interactions.

In spite of the daunting task of creating alternate hydrophobic regions in the protein interior, a number of attempts have yielded impressive results. The hydrophobic core of T4 lysozyme was altered without deleterious results by rational design. Several multiple mutants were made which destabilized the protein by less than 0.2 kcal/mol(42). Shuffling of residues in the hydrophobic core of a DNA binding protein resulted in mutants which retained partial activity(49). This experiment and another which modified λ repressor(36) suggest that the critical

determinant in these mutational studies is that the hydrophobic core remain hydrophobic.

Hydrogen Bonds

Not surprisingly, the contribution of hydrogen bonds upon protein stability has been widely debated. Hydrogen bonds have often been assumed to contribute little to protein stability. This was based upon the assumptions that there would be equal numbers of hydrogen bonds formed in the folded and unfolded states and that hydrogen bonds are energetically equivalent, with hydrogen bonds contributing primarily to specificity of folding. This theory has been questioned on the grounds that, in a protein, the ability to make and break hydrogen bonds is greatly reduced, resulting in an effective increase in the concentrations of hydrogen bonds(4).

The importance of hydrogen bonds can perhaps most accurately be assessed by two complementary approaches: The first is to analyze hydrogen bonds in folded proteins and determine what effect they might have in stabilizing the folded state of proteins. The second approach is site directed mutagenesis where hydrogen bonds are eliminated or hydrogen bonds are added where they did not previously exist. Site directed mutagenesis is often limited by steric constraints which often result in destabilization of the folded state.

An extensive study on the role of hydrogen bonding was undertaken on phage T4 lysozyme. Thr 157 was found to be important in the stabilization of T4 lysozyme. Substitution of Thr with Ile reduced the stability of lysozyme by approx

3 kcal/mol(29,31). Clearly, the size difference between Ile and Thr could not be ruled out as the dominating effect. However, Thr formed a hydrogen bond with the main-chain amide of Asp 159. Twelve additional mutants were created with substitutions at position 157(47). The five most stable mutagens all formed hydrogen bonds with the main chain amide nitrogen at Asp 159.

This study also showed that water can stabilize structures via ordered hydrogen bond formation. Gly 157 bound a water molecule in the crevice which resulted from its replacement of Thr and was nearly as stable as the native protein.

In another study involving phage T4 lysozyme, Pro 86 was substituted with 10 individual amino acids(4). Of these substitutions, Ser and Cys were shown crystallographically to form hydrogen bonds with the side chain of Gln 122. However, these mutants were no more stable than the mutants which did not form hydrogen bonds, suggesting that hydrogen bonds are not a panacea for protein stabilization. This raises a question central to the premise of this work; are some contributions to stability more important than others?

Secondary Structures

The two predominant secondary structures, α -helices and β -sheets are characterized by their main chain dihedral angles, Φ and Ψ . For α -helices, the average Φ and Ψ angles are approximately -60° and -50° respectively, which places them in the lower left-hand corner of a Ramachandran plot. For β -sheets,

the range of Φ - Ψ angles is much broader, and they fall into the upper left-hand quadrant of a Ramachandran plot.

α -Helices

The α -helix was first predicted in 1951 by Pauling(50). Using small-molecule crystal structures, he predicted the α -helix to be stable based upon geometrical factors. α -helices are characterized by 3.6 residues/turn with hydrogen bonds formed between C=O of residue n and the N-H group of residue $n + 4$. The rise per residue along the helix axis is approximately 1.5 Å. α -helices nearly always have a right-handed twist and the average length of an α -helix is 10 amino acids. Amphiphilicity, which is so often observed for α -helices, is a consequence of their preference for the protein surface, resulting in one side being embedded into the hydrophobic protein interior and the other exposed to aqueous solvent. The repeated hydrogen-bonds in α -helices orient all of the helical dipoles in the same direction resulting in a helical net dipole.

α -helices appear to be autonomously stable building blocks. This is supported by the crystal structure of melittin(10) and experiments which demonstrate the stability of isolated protein helices in water(46). As will be discussed, α -helices appear to play a major role in the stabilization of the heat stable thermolysin.

β -Sheets

β -sheets, by definition, are comprised of more than one β -strand. The orientation of the strands in a β -sheet can be parallel, antiparallel, or mixed, with bias against mixed β -sheets. The average length for a β -strand is 5 to 10 amino acids, with longer strands being more common in antiparallel sheets rather than in parallel sheets(11). Adjacent α -carbons alternate sides of the backbone and α -carbons two residues distant are separated by approximately 7 Å(51). β -sheets are characterized by a relatively flat surface on which to pack. There is a preference for side chains from groups adjacent to each other on neighboring strands to pair charged groups of opposite charge, to pair hydrophobic groups together, and to pair side chains branched at β -carbons with side chains which are unbranched in the β -carbon position(2).

Hydrogen bonding in β -sheets is much more directly aligned in antiparallel β -sheets than parallel β -sheets, which most likely contributes to the higher stability of antiparallel β -sheets. The nature of alignment of antiparallel β -sheets orients two adjacent, direct hydrogen bonds close to each other with a wider gap between these and the next set of hydrogen bonds. Parallel β -sheets are characterized by a more even distribution of diagonal hydrogen bonds. Both parallel and antiparallel sheets share the common trait of having an overall right-handed twist(21).

Parallel β -sheets almost always are comprised of at least five strands and these strands are generally removed from solvent on both sides(2). This is

contrasted to anti-parallel β -sheets which often consist of just two strands in which one side of the sheet is exposed to solvent. Both β -sheets display a tendency to be more hydrophobic in the central regions relative to end regions(23), resulting in central regions being embedded in the hydrophobic interior of the protein.

Motifs

Secondary structures combine to form motifs, regular identifiable patterns of protein structures. These motifs are influenced by a number of factors, such as constraints on their surface area and how different secondary structures pack. The packing is dominated by side-chains, which strive to close-pack. Three basic types of packing structures constitute the majority of packing observed in structural motifs. The combinations which are most common are helix-turn-helix, beta-turn-beta, and beta-alpha-beta structures. As their names imply, these motifs compose most of the methods of combining α -helices and β -sheets. While helix-turn-helix motifs clearly connect two α -helices, beta-turn-beta motifs commonly join two β -strands together in an antiparallel orientation, and beta-alpha-beta motifs are the building blocks of α/β open-twisted sheets and α/β barrels.

Beta-Alpha-Beta Motifs

In beta-alpha-beta structures, the α -helix packs nearly parallel to the β strands(26). The β -strands in α/β proteins average seven amino acids in length and α -helices average 14 residues in length. β -bulges are seldom found in these proteins. α -helices involved in beta-alpha-beta structures tend to be amphiphilic,

with the hydrophobic face packing against the β -sheets and the hydrophilic face projecting into the aqueous solvent.

Beta-Turn-Beta

Antiparallel β -sheets are often connected by β -hairpin turns and residues involved in these β -hairpins have a strong influence on which type of turn will be formed. Gly, Pro, and Asn play critical roles in turn types, as certain side-chains are not sterically allowed in some positions. The sheets formed from this arrangement invariably have one hydrophobic face.

Helix-Turn-Helix

Helix-turn-helix structures are common in proteins and suggest a structural role(2). The orientation of helices with respect to each other is dependent upon the residues which form the turn. As will be discussed, there are two basic patterns of packing which are formed from helix-turn-helix structures.

Side Chain Packing

α -Helices

The packing of helices and sheets is an intricate process which is determined by the side chains which protrude from the backbone. The factors influencing how side chains pack is the relative hydrophobicity, size and shape. Hydrophobic groups tend to be buried, while polar and charged groups prefer external positions. The size and shapes of the side-chains determine how well the

residues are able to accommodate close packing of the protein interior.

α -helices project a relatively flat face on which to pack with other secondary structures. Ridges are formed by residues separated by different numbers of residues in the primary sequence. The most common ridge involved in packing interactions is the one formed by residues $i, i+4, i+4n$. The next most commonly employed packing ridge is the one formed by residues $i, i+3, i+3n$. Finally, the packing ridge $i, i+1, i+1n$ is also observed. The preference seems to arise from the number of contact residues each ridge is capable of providing. Ridges formed by residues four distant in sequence do not rotate away from the packing face as quickly as those formed by either three or one residues distant, resulting in more contact atoms. Ridges which are formed by all small residues or all large residues form a topographically consistent ridge, while ridges which alternate large and small groups present a more varied ridge.

The packing of α -helices was first described by Crick in the early 1950s(1) in which he described the packing as knobs-into-holes. The ridge-groove packing vernacular is now more commonly used and will be employed in the rest of this text. A study of 50 helix-helix packing interactions(27) showed that the most common packing pattern was between two helices which both pack with their $i, i+4n$ ridges (4-4 packings), a pattern which was suggested to optimize the number of contacts between the helices. The angle between the two helical axes was generally estimated to be between -60° (51) and -52° (27), although the extremes were -27° and -74° . Not all packings of this type make equal numbers of contacts.

The total contacts are influenced by the residues which form the packing face, particularly the residues which are at the points where helices cross. Small residues at the crossing point seem to increase the numbers of contacts between α -helices by allowing more external residues to come into contact. The distances between helical axes was also reduced in these packings.

The next most commonly occurring packing pattern was a 3-4 packing. The angle between the helical axes averages $+23^\circ$ (27) and the number of contacts was determined to be less than in 4-4 packings, due to the larger curvature of these ridges away from the packing face. The number of residues involved in packing varied from six to 13. 4x4 and 3x4 crossed-ridge packing is made possible by a small residue on either one or both of the helices. The small residues are flanked by large residues. This forms a saddle in the helices which allows them to pack more closely. Crossing angles are approximately either $+40^\circ$ or -40° .

Helix-Sheet

There are two predominant classes of α -helices packing with β -sheets. The first type places the α -helices roughly antiparallel to the β -sheets. This type of packing pattern is characteristic of α/β barrels and α/β open twisted sheets where amphiphilic α -helices employ their hydrophobic faces to protect hydrophobic regions of β -sheets. The natural twist of β -sheets places the residues at the ends of the β strand farther away from residues in the helix(51). The other major type of helix-sheet packing interaction occurs when α -helices cross β -sheets. In these instances, the contact residues from the α -helices are from two adjacent $\pm 4i$

rows(26). With respect to adjacent strands in a β -sheet, if residues i and j are next to each other, residue i from the first strand and residue $j+2$ contact the α -helix.

Sheet-Sheet

When β -sheets pack with each other, there is a strong preference for the sheets to pack at an angle which is not parallel, a result of the drive for optimal packing interactions. When residues from the opposing sheets are approximately the same size, the packing has been stated to resemble a bilayer structure(26). However, when a large residue from the first sheet interacts with small residues from the second sheet, the larger residue is more accurately viewed as interdigitating with the smaller residues.

Computer Programs

Computer programs used in the study of proteins fall into two main categories, predictive and analytical. Predictive programs attempt to predict the secondary structure or the folded state of a protein from the primary sequence. Analytical programs study the interactions which take place within proteins. These two different applications of the power of computers will be addressed separately.

Predictive Programs

The prediction of protein secondary structure has not improved drastically since Chou and Fasman first published a statistical analysis on the probable

occurrences of amino acids in helices and sheets(6). Much of tertiary structure prediction has focused on prediction of secondary structure and then the positioning of secondary structures into an approximated tertiary fold. Basic strategies for the prediction of protein secondary structure are listed in the following paragraphs.

The first is a pattern matching method which is based upon hydrophobic and hydrophilic sequences which are characteristic of certain secondary structures. Another method was devised which sought more intricate patterns, based upon characteristic patterns such as the positioning of unlike charge groups four residues distant in an α -helix.

Chou and Fasman(6) devised a statistical method based upon the occurrence of amino acids in different secondary structural motifs. The success rate of this method was slightly greater than 50%. Chou and Fasman found weak preferences for some amino acids. They found Ala, Glu, Leu, and Met to be common in α -helices, while Gly, Pro, Ser, and Tyr are the least likely amino acids to form α -helices.

Neural networks have been designed to recognize patterns and these programs modestly increase the accuracy of secondary structure prediction(15).

Tertiary structure prediction methods tend to be more intricate. These generally take into account long range interactions between residues(33) and some go so far as to predict side chain conformation through packing optimization(37).

An interesting strategy of structure prediction is the approach of the inverse

folding problem. This method attempts to match sequences to a given three dimensional structure(52) or "tertiary template".

An assumption of tertiary templates is that a set of internal residues, not sequentially related, defines the structural motif. All other residues are assumed to be external and affect the structure only permissively through the global free energy(32). Electrostatic or other properties determine whether folding will occur.

A promising tool for homology modeling is one which ranks amino acids according to their affinity for buried hydrophobic positions, partially buried polar positions, or exposed external positions(48). Given a three-dimensional structure, a sequence is given an overall score according to how well it is capable of fitting the tertiary structure. It has been successful in the prediction of globin fold proteins.

A unique method of structure prediction looks at the mechanical properties of proteins while ignoring quantum mechanical aspects of protein folding(35). In this work, helices are considered to be rigid rods and loops are considered to be elastic units. The stress which loops place upon different packing patterns is then measured. In an application of this method, all combinations of packing of the helices of myoglobin were studied and the native structure was found to be the least stressed.

Quantum mechanical and thermodynamical methods for the prediction of the folded state of proteins have not yet become feasible. The computer time necessary to apply these methods is prohibitive as the time scale upon which they

work is on the picosecond scale while folding generally occurs on the scale of milliseconds to minutes.

In energy minimization(61), the potential energy of a system is generally treated as a function of the atomic positions and is given by an equation of the form: $E = E_b + E_\theta + E_\Phi + E_{vdw} + E_{es}$

where b is bond stretching, θ is bond angle bending and Φ is rotation around a bond. vdw and es represent van der Waals contributions and electrostatic contributions. The main limitation of energy minimization is that thermal motions are not taken into account and therefore, entropic effects are not simulated. Structures often fall into false energy minima.

Molecular dynamics is an algorithm for numerically solving the equations of motion. Each of the atoms in the potential energy equation is taken as a point mass and Newton's laws are applied. The equations which result contain the necessary information to determine the positions of each atom as a function of time.

Analytical Programs

Most analytical programs either look at patterns of interactions between amino acids, without regard to secondary structure, or look at intra-secondary structure interactions. For example, the pattern ala-ala-x-x-lys was found to occur predominantly in α -helices while val-x-val-x-x-x-ala occurred either in a β strand or an extended structure(34). Recently, the work of Richardson(63) has shown amino acid preferences for the terminal amino and carboxyl positions of helices

while others have shown that stabilization of the backbone dipole at the ends of helices can also stabilize α -helices(64).

The method of measuring the solvent accessibility of residues and atoms in a protein has been popular since the original work of Richards(19). It was found that an average of two completely buried ionizable groups per protein occurred and that 20% of the ionizable groups did not form salt-bridges(30). However, the groups which did not form salt-bridges all formed hydrogen bonds. There is a strong preference for salt-bridges to be involved in active sites. The charged amine groups of Lys and Arg were found to be the least likely to occur in the protein interior.

In an extension of this work, surface charge density and overall charge density were measured on a variety of proteins(13). Not surprisingly, the charge density in active sites was higher than other regions of the protein. However, surface charge density did not vary dramatically for any of the observed proteins and only varied between one and two charged groups per 100 $\text{\AA}^2$.

In investigations of the packing of side chains, densities were measured for side chains atoms within 4.5 $\text{\AA}$ of all side-chain atoms. Clusters of charged groups were found to occur near the protein surface and often near the amino- or carboxy-terminus(39). This study, as well as another which looked at hydrocarbon contacts within a 5.2 $\text{\AA}$ radius(43), did not analyze these results according to how it applied to the interaction between secondary structures. Another study, which looked at the interactions between amino acids (with no analysis of secondary

structures), found the usual preferences for hydrophobic side chains to interact with hydrophobic side chains and not with charged groups(16). Other programs have searched crystal structures for regions which have similar backbone topology in an attempt to find structural similarities(40).

STATEMENT OF THE PROBLEM

There remains a lack of detailed information as to the patterns of how secondary structures interact in folded proteins. This work represents an initial attempt to develop a system to profile proteins which can then be useful in protein structure prediction and the design of novel proteins. A number of programs have been written in this study which analyze the interactions between protein residues. These programs range from those which analyze total interactions to those which analyze interactions between secondary structures, which in this work are considered to be comprised only of α -helices and β -sheets.

A logical approach, which has been devised in this work, is to look at interactions between secondary structures with respect to the backbone atoms which are in closest contact between the two secondary structures. For the determination of nearest contact, only the backbone C, N, and C- α atoms are considered. All of the rest of the interacting residues between these two secondary structures are then numbered according to their respective positions to these atoms. Residues which have higher sequence numbers are given positive numbers and those with lower sequence numbers are given negative numbers.

As has been discussed, the packing patterns of different secondary structure interactions affect the angles at which these secondary structures cross. The angles between secondary structures are also measured in this work and

interactions are also analyzed with crossing angles taken into account. Programs have been written which determine direction vectors of helix and sheet axes and then compute the angles between the secondary structures.

Eleven types of atom-atom interactions are considered in this work. These interactions are hydrophobic side chain atoms with other hydrophobic side chain atoms, hydrophobic side chain atoms with backbone atoms, backbone atoms with backbone atoms, polar side chain atoms with polar side chain atoms, polar side chain atoms with backbone amide nitrogen atoms, polar side chain atoms with backbone carbonyl oxygen atoms, charged atoms with polar side chain atoms, charged atoms with backbone amide nitrogen atoms, charged atoms with backbone carbonyl oxygen atoms, charged atoms with oppositely charged atoms, and charged atoms with atoms of like charge.

The aforementioned programs have been applied to 67 proteins. Profiles of individual proteins as well as overall tendencies have been computed. Additionally, the thermally stable thermolysin is analyzed in an effort to determine if heat stable proteins have preferences for certain types of interactions. A premise of this work is that not all interactions are equal and hypotheses are formed as to which interactions have a greater effect upon stability.

EXPERIMENTAL

Selection of Database

Strategy

It became necessary to develop a system which would efficiently handle programs required to run on 67 individual proteins. This was accomplished using the *emacs* editor. Macro commands were employed to set up command jobs which were then executed by shell commands. Raw data was obtained from the 1992 Brookhaven Protein X-ray Crystallography databank utilizing the UNIX system. While in the Brookhaven directory, a listing of all sequences was obtained. The UNIX emacs editor was employed to create a shell file. A shell file allows repetitive commands to be processed by the computer, which results in increased efficiency in the processing of data. The following macro was then written and inserted prior to each row in the temp file:

```
grep "REMARK 2 RESOLUTION" /usr/brookhaven/filename
```

These commands were issued to the computer and the output was redirected to a separate file. Data were then sorted by use of a UNIX sort command in ascending order. The emacs editor was again employed to remove files with resolutions greater than 2 Å, files resolved under 2.0 Å which contained qualifier statements, and files which did not list a resolution. This resulted in 376 files

which met the qualification of 2 Å resolution or better. After removal of DNA structures and multiple phage T4 lysozyme mutants, 249 files remained.

The next objective was to take all structures which had 2 Å resolution or better and determine which structures had been refined to r-factors less than or equal to 0.20. The following grep command was issued to determine the refinement factors of the structures in question:

```
grep "REMARK 3" /usr/brookhaven/filename
```

The output from this command was then edited in emacs for structures with refinement factors which met the criterion. This reduced the number of structures to 188 entries.

The next objective was to sort the output from the previous command to remove different crystal structures of the same protein, and mutant protein structures obtained primarily through genetic engineering. Of the previous files, 134 files were examined to determine uniqueness. Structures often differed in the binding of a cofactor or an inhibitor. In these cases, structures were chosen which most resembled the native unbound protein. The number of proteins which met the requirement of uniqueness were 67. This represented the source file which was used in the following assessment of the databank.

A list of the 67 files used in this work follows: 1aap (protease inhibitor domain of alzheimer's amyloid), 1apb (l-arabinose-binding protein), 1bbp (bilin binding protein), 1bp2 (phospholipase a), 1ca2 (carbonic anhydrase), 1ccr (cytochrome c), 1cdp (parvalbumin b), 1cho (alpha-chymotrypsin), 1cox

(cholesterol oxidase), 1csc (citrate synthase), 1ctf (ribosomal protein), 1gct (gamma-chymotrypsin a), 1gp1 (glutathione peroxidase), 1hmd (hemerythrin), 1hoe (alpha-amylase inhibitor), 1i1b (interleukin-1), 1lyd (phage t4-lysozyme), 1mba (myoglobin), 1omd (oncomodulin), 1pal (parvalbumin), 1pcy (plastocyanin), 1ppd (2-hydroxyethylthiopapain), 1r69 (434 repressor), 1rbp (retinol binding protein), 1rnk (selenomethionyl ribonuclease h), 1rsm (ribonuclease), 1s02 (subtilisin bpn'), 1sar (ribonuclease sa), 1sgt (trypsin), 1snc (staphylococcal nuclease), 1tgs (trypsinogen), 1tld (beta-trypsin), 1tmn (thermolysin), 1ton (tonin), 1ubq (ubiquitin), 21bi (interleukin-1 beta), 256b (cytochrome b562), 2apr (acid proteinase), 2c2c (cytochrome c), 2cab (carbonic anhydrase), 2ci2 (chymotrypsin inhibitor 2), 2cpp (cytochrome p450), 2fcr (flavodoxin), 2gbp (d-galactose/d-glucose binding protein), 2hhb (hemoglobin), 2mlt (melittin), 2ovo (ovomucoid), 2paz (pseudoazurin), 2prk (proteinase k), 2ptc (beta-trypsin), 2rhe (bence-jones protein), 2rsp (rous sarcoma virus protease), 2sec (subtilisin carlsberg), 2tim (triosephosphate isomerase), 2tsc (thymidylate synthase), 2utg (uteroglobin), 2wrp (trp repressor), 351c (cytochrome c-551), 3app (acid proteinase), 3bcl (bacteriochlorophyll-a protein), 3blm (beta-lactamase), 3cla (type /iii chloramphenicol acetyltransferase), 3dfr (dihydrofolate reductase), 3grs (glutathione reductase), 4fxn (flavodoxin), 4pep (pepsin), 4pti (trypsin inhibitor).

Core Programs

The following programs count contacts between atoms and constitute the core of the programs. In this work, the terms interactions and contacts are used interchangeably. All programs in this work, were written in the "C" programming language. The outputs are given in number of atom-atom contacts for each residue pair in contact. For programs involving hydrophobic atoms, the contact distance is set as the sum of the van der Waal radii + 0.4 Å. The choices for van der Waal radii were taken from the ACCESS program which was provided by Fred Richards. The 0.4 Å distance can be modified by changing the CUTOFF value. For polar and charged groups, the distance between the two groups can be modified in the DIPOLEDIST or CHARGEDIST values. The default settings used in this work were 3.25 Å for dipole-dipole interactions, 3.75 Å for charge-dipole interactions, and 5.0 Å for charge-charge interactions. All of these programs run on Brookhaven databank files and do not require modification unless identical dimers are to be eliminated.

Backbone - Backbone Contacts

This program counts contacts between backbone atoms. Backbone atoms were selected to be C, C_α, N, and O for this program. The output for this program and all of the core programs which follow list the names of the interacting residues, the residue numbers of interacting residues, the protein's Brookhaven filename, the subunits that the residues belong to (if any), and the number of atom-atom

contacts which are made.

Backbone - Hydrophobic Side Chain Contacts

The number of contacts were counted between hydrophobic side chain atoms and the backbone atoms C, C_α, N, and O.

Hydrophobic Side Chain - Hydrophobic Side Chain Contacts

This program counts the number of atom-atom contacts between hydrophobic side chain atoms. In this study, all side chain atoms except nitrogen and oxygen atoms are considered to be hydrophobic. This includes the sulfhydryl groups of both Cys and Met. A partial output of this file is given in Table 1.

Charged - Polar Side Chain Contacts

Contacts between charged atoms and polar side chain atoms within 3.75 Å are counted by this program.

Charged - Backbone Carbonyl Oxygen Contacts

This program counts all contacts within 3.75 Å between charged atoms and backbone carbonyl atoms.

Charged - Backbone Amide Nitrogen Contacts

Contacts within 3.75 Å between charged atoms and backbone carbonyl atoms are counted by this program.

Table 1. Sample output from the program Hydrophobic Side-Chain - Hydrophobic Side-Chain Contacts for thermolysin.

BROOKHAVEN FILENAME	RESIDUE 1 NAME & NUMBER		RESIDUE 2 NAME & NUMBER		NUMBER OF CONTACTS	CHAIN I.D.	
						1	2
1TMN	ILE	1	THR	23	1	E	E
1TMN	ILE	1	SER	25	1	E	E
1TMN	ILE	1	TYR	29	8	E	E
1TMN	ILE	1	LEU	54	1	E	E
1TMN	THR	4	THR	6	1	E	E
1TMN	THR	4	TYR	24	3	E	E
1TMN	THR	6	THR	4	1	E	E
1TMN	THR	6	TYR	24	1	E	E
1TMN	VAL	7	ASN	19	1	E	E
1TMN	VAL	9	PHE	63	3	E	E
1TMN	VAL	9	GLN	17	2	E	E
1TMN	AR	11	PHE	63	2	E	E
1TMN	VAL	13	ILE	131	2	E	E
1TMN	VAL	13	PRO	132	3	E	E
1TMN	VAL	13	ALA	68	1	E	E
1TMN	LEU	14	ILE	131	1	E	E
1TMN	LEU	14	ASP	191	1	E	E
1TMN	ASP	16	LYS	18	1	E	E
1TMN	GL	17	VAL	9	2	E	E
1TMN	LYS	18	TYR	75	6	E	E
1TMN	LYS	18	VAL	71	2	E	E
1TMN	LYS	18	ASP	16	1	E	E
1TMN	AS	19	VAL	7	1	E	E
1TMN	ILE	20	HIS	74	1	E	E
1TMN	ILE	20	THR	22	1	E	E
1TMN	ILE	20	VAL	71	2	E	E
1TMN	ILE	20	TYR	75	2	E	E
1TMN	ILE	20	LEU	30	1	E	E
1TMN	ILE	20	PHE	62	2	E	E
1TMN	AS	21	ASP	32	2	E	E
1TMN	THR	22	ILE	20	1	E	E
1TMN	THR	22	LEU	30	1	E	E
1TMN	THR	22	PHE	62	2	E	E
1TMN	THR	23	GLN	31	1	E	E
1TMN	THR	23	ILE	1	1	E	E
1TMN	TYR	24	THR	4	3	E	E
1TMN	TYR	24	THR	6	1	E	E
1TMN	TYR	24	TYR	28	10	E	E
1TMN	SER	25	ILE	1	1	E	E
1TMN	TYR	27	TYR	29	1	E	E
1TMN	TYR	27	ALA	56	1	E	E
1TMN	TYR	28	ASN	60	9	E	E
1TMN	TYR	28	TYR	24	10	E	E
1TMN	TYR	29	GLN	31	1	E	E
1TMN	TYR	29	LEU	54	4	E	E

Polar Side Chain - Polar Side Chain Contacts

This program counts contacts between polar side chain atoms which are within 3.25 Å of each other.

Polar Side Chain - Backbone Carbonyl Oxygen Contacts

This program counts all contacts within 3.25 Å between polar side chain atoms and backbone carbonyl atoms.

Polar Side Chain - Backbone Amide Nitrogen Contacts

Contacts within 3.75 Å between polar side chain atoms and backbone carbonyl atoms are counted by this program.

Oppositely Charged Atom Contacts

In this program, all oppositely charged atom interactions which are less than 5.0 Å are considered. Amino-terminal N atoms and carboxy-terminal O atoms are included in the measurements.

Like Charged Atom Contacts

This program counts all interactions between atoms of the same charge which are within 5 Å of each other. As with the previous program, amino-terminal N atoms and carboxy-terminal O atoms are included in the measurements.

Angle Determination

The next set of programs are involved in the determination of crossing angles between secondary structures. Four individual programs were written to accomplish this end and each of the programs served a distinct function. In these programs, the direction vectors of the secondary structures were taken to start at the amino-terminus and run toward the carboxy-terminus.

The objective was to write programs which would accomplish the following:

The direction vector of one of the secondary structures is projected onto the y-axis with its direction vector pointing in the positive y direction. Its x and z components are set equal to zero. The manipulations required to accomplish this are performed on the vector for the other secondary structure in question. Next, looking down the z-axis, it is determined which of the vectors crosses in front of the other, i.e., which vector has a more positive z value at the point of crossing. If the initial vector lies in front of the second vector, the angle is determined without further modifications. However, if the second vector crosses in front of the initial vector, the system is rotated 180° about the y-axis and the angle is determined. When determining the angle, the origins of both vectors are placed upon the origin of the Cartesian coordinate system. The first vector, as has been determined projects upward on the y-axis. The angles are then measured with respect to the x-y plane. When viewing the angle between the two vectors, if the second vector is rotated in the clockwise direction and the angle is less than or equal to 180° , the angle is considered to be positive. If the second vector is

rotated in the counterclockwise direction and less than 180° , the angle is considered to be negative. The following is a description of the four programs designed to calculate angles between secondary structures.

Angle

The requirements of this program were two-fold; initially, direction vectors for helices and sheets were determined and then angles between secondary structures were determined. Residues involved in secondary structures were read in from the Brookhaven files. Only α -helices comprised of five or greater residues and β -sheets comprised of three or greater residues were considered to be secondary structures.

The direction vector for β -sheets was determined as follows: 1) the midpoint of the β -sheet was calculated by adding the upper boundary and the lower boundary and then dividing by two, 2) the x, y, and z coordinates for the α -carbon one residue prior to the midpoint was subtracted from the x, y, and z coordinates of the α -carbon one residue past the midpoint.

For α -helices, the midpoint was determined in the same way. The strategy for determining the direction vector consisted of three separate steps. The first step was to calculate two vectors, both of which were orthogonal to the axis of the α -helix. The second step was to find the vector which was orthogonal to both of the first two vectors. This vector was parallel to the axis of the helix. The third step determined the actual direction of the vector, as the first two steps could produce a vector which was parallel to the direction vector, but in the opposite

direction.

The first orthogonal vector was determined in the following manner (all coordinates are for α -carbons; positions are relative to the midpoint of the helix, eg. $M-2(x)$ represents the x coordinate of the α -carbon two residues toward the amino-terminus of the α -helix from the midpoint of the α -helix):

$$\text{vector1}(x) = M-2(x) + M(x) - 2(M-1(x))$$

$$\text{vector1}(y) = M-2(y) + M(y) - 2(M-1(y))$$

$$\text{vector1}(z) = M-2(z) + M(z) - 2(M-1(z))$$

The second orthogonal vector was determined analogously, starting one residue further toward the carboxy-terminal end of the α -helix:

$$\text{vector2}(x) = M-1(x) + M+1(x) - 2(M(x))$$

$$\text{vector2}(y) = M-1(y) + M+1(y) - 2(M(y))$$

$$\text{vector2}(z) = M-1(z) + M+1(z) - 2(M(z))$$

The vector which is orthogonal to both of the first two vectors is calculated by taking the cross-product of the components of the first two vectors:

$$\text{vector3}(x) = \text{vector1}(y) \times \text{vector2}(z) - \text{vector1}(z) \times \text{vector2}(y)$$

$$\text{vector3}(y) = \text{vector1}(z) \times \text{vector2}(x) - \text{vector1}(x) \times \text{vector2}(z)$$

$$\text{vector3}(z) = \text{vector1}(x) \times \text{vector2}(y) - \text{vector1}(y) \times \text{vector2}(x)$$

vector3 is parallel to the helical axis. To determine if this vector is actually in the correct direction, the following strategy was devised: First, a crude direction vector was determined for the α -helix in question. Then the angle(Θ) between the crude direction vector and vector3 was computed. If Θ was less than $\pi/2$, the

value for vector3 was left unchanged. If Θ was greater than $\pi/2$, the x, y, and z values for vector3 became the negative value of their original values. The crude direction vector was determined as follows:

$$\text{vector4}(x) = M+2(x) - M-2(x)$$

$$\text{vector4}(y) = M+2(y) - M-2(y)$$

$$\text{vector4}(z) = M+2(z) - M-2(z)$$

This step assigned a vector which began at one α -carbon and proceeded to the α -carbon four residues toward the carboxyl-end of the helix. This is a rough approximation of the direction of the helical axis.

The computations for theta are as follows:

$$\begin{aligned} \theta = \arccos & \left(\frac{(\text{vector4}(x) \times \text{vector3}(x) + \text{vector4}(y) \times \text{vector3}(y) + \right. \\ & \left. \text{vector4}(z) \times \text{vector3}(z)) \cdot ((\text{vector3}(x))^2 + (\text{vector3}(y))^2 + \right. \\ & \left. (\text{vector3}(z))^2)^{1/2} \times ((\text{vector4}(x))^2 + (\text{vector4}(y))^2 + \right. \\ & \left. (\text{vector4}(z))^2)^{1/2}} \right) \end{aligned}$$

At this point, the angle between the two secondary structures has been computed. The remainder of the programs determine whether the angle is positive or negative. The output for this program contains the name of the Brookhaven file, whether the secondary structures are helices or sheets, the angle between the secondary structures, and the lower and upper boundaries of the secondary structures.

Nearest-Backbone-Contact

This program measures the atoms from each secondary structure which are in closest contact. Only the backbone atoms C, C _{α} , and N are considered in this measurement. The carbonyl O atom is omitted, since it projects out from the cylinder of the α -helix and would bias the results. The results from this program are used in the final program in which the sign of the angle is computed. The output consists of the backbone atom names which are in nearest contact, the residue names for the atoms which are in nearest contact, the residue numbers for the atoms which are in nearest contact, the lower and upper boundaries of the secondary structures involved, whether the secondary structures involved are helices or sheets, the subunits which the contacts belong to (if any), and the contact distance for the atoms which are in nearest contact.

Angle-Nearest-Backbone-Combine

The output from the previous two programs are combined in this program. The output from this program becomes part of the input for the next program.

Angle-Sign-Determination

The final step in this set of programs is to determine whether the angle is positive or negative. The success of this program relies on the ability to correctly assess the relative positions of the two secondary structures in space as they cross. This does not appear to be a concern for β -sheets. However, α -helices are more problematic. The difficulties arise because nearest backbone atom contacts

are used to determine the relative positions of the secondary structures rather than the actual axes of the helices. In effect, the initiation points of helical axes are at backbone atom positions. This method has the potential to incorrectly determine the positions of axes as they cross. The evolution of the strategies for the determination of the sign of crossing angles will be outlined.

The initial strategy ignored the z component of the direction vectors for the two secondary structures. Rather, it was determined which of the backbone atoms in nearest contact had a more positive z value. If the initial vector from the first program was more positive, the angles between a vector which represents the y-axis in the positive y direction and the x and y components of the respective direction vectors were measured. Next, the angle between the initial direction vector and the y-axis was subtracted from the angle between the second direction vector and the y-axis. If this value was either greater than 0° and less than or equal to 180° or less than -180° , the sign of the angle was considered to be positive. However, if this value was either less than 0° and greater than -180° or greater than 180° , the sign of the angle was considered to be negative.

This initial attempt correctly assigned the sign of the crossing angles for most of the secondary structures which were tested. However, occasionally the z coordinates for the backbone atoms in nearest contact were close in value and the relative positions of the secondary structures were reversed, resulting in incorrect assignments for the signs of the crossing angles. In an attempt to remedy this, rather than considering only the z coordinates of the nearest

backbone atoms, the coordinates which possessed greatest difference between coordinate values were employed. When the difference between x coordinates was larger than the difference between either the y or z coordinates, the z-axis became the reference axis and the angles were determined with respect to the y-z plane. If the difference between the z coordinates was larger than the difference between either the x coordinates or y coordinates, the x-axis became the reference axis and the angles were determined with respect to the x-z plane.

This program correctly assigned the sign of the crossing angles for nearly all of the secondary structures which were tested. The only failures which were observed were in α -helices which were contiguous. In these instances, the nearest backbone atoms would occasionally result in incorrect assignments for the relative positions of the secondary structures and the concomittal incorrect assignment of the sign of the angles. To circumvent this problem, a value for coordinates of the nearest backbone atoms was determined to be the average value of the coordinates of four α -carbons in the vicinity of the nearest backbone atom. This gave x, y, and z coordinate values which more correctly approximated the axis of the helix. The program was written so that only α -carbons which were part of the helices in question were considered. The program followed the same protocol from this point forward as the prior program. This program correctly assigned the sign for all secondary crossing angles in both hemoglobin and thermolysin.

These programs require the atom.h file be present in the working directory.

atom.h is a library file used to store common blocks of information in order to reduce the amount of memory used by the programs.

Programs Which Combine Data

Several of the following programs require an input file which contains the residue contact information, the crossing angles between secondary structures, and the nearest backbone contacts. For some of the later programs, it is necessary to modify the Brookhaven data file if it contains more than one listing of the same β -strand. This is occasionally the case, when the authors list the same strand as belonging to more than one sheet. The following programs combine data:

Combine

This program combines output from a core program and the final program for assigning the correct sign to the secondary structure crossing angles. The output consists of the number of atom-atom contacts, the Brookhaven file name, whether each of the secondary structures is either a helix or a sheet, residue names of residues in contact, residue numbers of residues in contact, the angles between secondary structures, the lower and upper boundaries for each of the secondary structures, the nearest contact backbone atoms, the residue numbers of the nearest contact backbone atoms, and which subunit the interacting residues belong to. A partial output of this program for thermolysin is given in Table 2.

Table 2. Sample output from the program Combine for thermolysin.

SECONDARY STRUCTURE			NEAREST BACKBONE CONTACT				POSITION	
1	2	BROOKHAVEN FILENAME	RESIDUE 1	RESIDUE 2	ATOM 1	ATOM 2	RESIDUE 1	RESIDUE 2
SHEET	SHEET	1TMN	8	20	C	N	-4	4
SHEET	SHEET	1TMN	8	20	C	N	-2	4
SHEET	SHEET	1TMN	8	20	C	N	-1	-1
SHEET	SHEET	1TMN	8	20	C	N	1	-3
SHEET	SHEET	1TMN	20	8	N	C	-3	1
SHEET	HELIX	1TMN	20	75	CA	CA	-2	0
SHEET	HELIX	1TMN	20	75	CA	CA	-2	-4
SHEET	SHEET	1TMN	20	8	N	C	-1	-1
SHEET	HELIX	1TMN	20	75	CA	CA	0	-1
SHEET	HELIX	1TMN	20	75	CA	CA	0	-4
SHEET	HELIX	1TMN	20	75	CA	CA	0	0
SHEET	SHEET	1TMN	20	8	N	C	4	-4
SHEET	SHEET	1TMN	20	8	N	C	4	-2
SHEET	SHEET	1TMN	25	27	C	N	-1	1
SHEET	SHEET	1TMN	28	57	C	N	-1	-1
SHEET	SHEET	1TMN	27	25	N	C	1	-1
SHEET	SHEET	1TMN	29	54	CA	C	0	0
SHEET	SHEET	1TMN	28	57	C	N	1	-1
SHEET	SHEET	1TMN	42	102	N	C	-3	-2
SHEET	HELIX	1TMN	41	74	CA	CA	-2	0
SHEET	HELIX	1TMN	41	74	CA	CA	-2	3

Table 2. Sample output from the program Combine for thermolysin (continued).

SECONDARY STRUCTURE RANGES				CONTACT RESIDUES		CROSSING ANGLE	BACKBONE SEPARATION DISTANCE	NUMBER CONTACT	CHAIN I.D.	
LOWER 1	UPPER 1	LOWER 2	UPPER 2	RESIDUE 1	RESIDUE 2				1	2
2	11	16	25	THR	TYR	169.35	3.77	3	E	E
2	11	16	25	THR	TYR	169.35	3.77	1	E	E
2	11	16	25	VAL	ASN	169.35	3.77	1	E	E
2	11	16	25	VAL	GLN	169.35	3.77	2	E	E
16	25	2	11	GLN	VAL	169.35	3.77	2	E	E
16	25	65	87	LYS	TYR	71.418	6.17	6	E	E
16	25	65	87	LYS	VAL	71.418	6.17	2	E	E
16	25	2	11	ASN	VAL	169.35	3.77	1	E	E
16	25	65	87	ILE	HIS	71.418	6.17	1	E	E
16	25	65	87	ILE	VAL	71.418	6.17	2	E	E
16	25	65	87	ILE	TYR	71.418	6.17	2	E	E
16	25	2	11	TYR	THR	169.35	3.77	3	E	E
16	25	2	11	TYR	THR	169.35	3.77	1	E	E
16	25	27	29	TYR	TYR	136.957	3.16	10	E	E
27	29	55	57	TYR	ALA	104.569	3.89	1	E	E
27	29	16	25	TYR	TYR	136.957	3.16	10	E	E
27	29	52	54	TYR	LEU	-129.054	6.07	4	E	E
27	29	55	57	TYR	ALA	104.569	3.89	2	E	E
39	43	100	106	ILE	ILE	-14.149	3.99	1	E	E
39	43	65	87	ILE	HIS	162.757	5.89	1	E	E
39	43	65	87	ILE	ALA	162.757	5.89	1	E	E

Secondary-Structure-Total-Combine

This program combines output from the same programs as Combine. The difference is that the output is given for total interactions (residue-residue contacts, atom-atom contacts and the ratio of atom-atom contacts/residue-residue contacts) between two secondary structures. The output does not list the residue names or residue numbers of individual interactions as can be seen for the partial output of this program in Table 3.

Range

This program takes the output from the program Combine and classifies the contacts according to the angle ranges of the secondary structures. The angle ranges are 30° increments starting at 0° and covering both positive and negative angle values. In order to further increase the fidelity of this program, individual interactions are also listed for additional angle ranges which are offset by 15° from the previous ranges. A sample output is listed in Table 4.

Total-Residue Pair-Interactions

This program takes the output from any Core program and computes the total number of interactions between each residue pair (e.g. Ala-Leu) as well as the average number of atom-atom contacts for each interacting residue pair.

Secondary Structure-Residue Pair-Interactions

The output for this program is the same as the previous program. However,

Table 3. Sample output from the program Range for thermolysin.

SECONDARY STRUCTURE		BROOKHAVEN FILENAME	NEAREST BACKBONE CONTACT				POSITON	
1	2		RESIDUE 1	RESIDUE 2	ATOM 1	ATOM 1	RESIDUE 1	RESIDUE 2
SHEET	SHEET	1TMN	8	20	C	N	-4	4
SHEET	SHEET	1TMN	8	20	C	N	-4	4
SHEET	SHEET	1TMN	8	20	C	N	-2	4
SHEET	SHEET	1TMN	8	20	C	N	-2	4
SHEET	SHEET	1TMN	8	20	C	N	-1	-1
SHEET	SHEET	1TMN	8	20	C	N	-1	-1
SHEET	SHEET	1TMN	8	20	C	N	1	-3
SHEET	SHEET	1TMN	8	20	C	N	1	-3
SHEET	SHEET	1TMN	20	8	N	C	-3	1
SHEET	SHEET	1TMN	20	8	N	C	-3	1
SHEET	HELIX	1TMN	20	75	CA	CA	-2	0
SHEET	HELIX	1TMN	20	75	CA	CA	-2	0
SHEET	HELIX	1TMN	20	75	CA	CA	-2	-4
SHEET	HELIX	1TMN	20	75	CA	CA	-2	-4
SHEET	SHEET	1TMN	20	8	N	C	-1	-1
SHEET	SHEET	1TMN	20	8	N	C	-1	-1
SHEET	HELIX	1TMN	20	75	CA	CA	0	-1
SHEET	HELIX	1TMN	20	75	CA	CA	0	-1
SHEET	HELIX	1TMN	20	75	CA	CA	0	-4
SHEET	HELIX	1TMN	20	75	CA	CA	0	-4
SHEET	HELIX	1TMN	20	75	CA	CA	0	0

Table 3. Sample output from the program Range for thermolysin (continued).

SECONDARY STRUCTURE RANGES				CONTACT RESIDUES		CROSSING ANGLE	ANGLE RANGE		BACKBONE SEPARATION DISTANCE	NUMBER CONTACT	CHAIN I.D.	
LOWER 1	UPPER 1	LOWER 2	UPPER 2	RESIDUE 1	RESIDUE 2		LOWER	UPPER			1	2
2	11	16	25	THR	TYR	169.35	150	180	3.77	3	E	E
2	11	16	25	THR	TYR	169.35	165	-165	3.77	3	E	E
2	11	16	25	THR	TYR	169.35	150	180	3.77	1	E	E
2	11	16	25	THR	TYR	169.35	165	-165	3.77	1	E	E
2	11	16	25	VAL	ASN	169.35	150	180	3.77	1	E	E
2	11	16	25	VAL	ASN	169.35	165	-165	3.77	1	E	E
2	11	16	25	VAL	GLN	169.35	150	180	3.77	2	E	E
2	11	16	25	VAL	GLN	169.35	165	-165	3.77	2	E	E
16	25	2	11	GLN	VAL	169.35	150	180	3.77	2	E	E
16	25	2	11	GLN	VAL	169.35	165	-165	3.77	2	E	E
16	25	65	87	LYS	TYR	71.42	60	90	6.17	6	E	E
16	25	65	87	LYS	TYR	71.42	45	75	6.17	6	E	E
16	25	65	87	LYS	VAL	71.42	60	90	6.17	2	E	E
16	25	65	87	LYS	VAL	71.42	45	75	6.17	2	E	E
16	25	2	11	ASN	VAL	169.35	150	180	3.77	1	E	E
16	25	2	11	ASN	VAL	169.35	165	-165	3.77	1	E	E
16	25	65	87	ILE	HIS	71.42	60	90	6.17	1	E	E
16	25	65	87	ILE	HIS	71.42	45	75	6.17	1	E	E
16	25	65	87	ILE	VAL	71.42	60	90	6.17	2	E	E
16	25	65	87	ILE	VAL	71.42	45	75	6.17	2	E	E
16	25	65	87	ILE	TYR	71.42	60	90	6.17	2	E	E

Table 4. Sample output from the program Secondary Structure Total Combine for thermolysin.

SECONDARY STRUCTURE		BROOKHAVEN FILENAME	SECONDARY STRUCTURE RANGES				NEAREST BACKBONE CONTACT					
1	2		LOWER 1	UPPER 1	LOWER 1	UPPER 1	RESIDUE NAMES		RESIDUE NUMBERS		ATOM NAMES	
							RESIDUE 1	RESIDUE 2	NUMBER 1	NUMBER 2	ATOM 1	ATOM 2
HELIX	HELIX	1TMN	65	87	137	150	THR	ALA	80	141	CA	CA
HELIX	HELIX	1TMN	65	87	160	180	THR	VAL	80	176	CA	CA
HELIX	SHEET	1TMN	65	87	39	43	HIS	THR	74	41	CA	CA
HELIX	SHEET	1TMN	65	87	100	106	PRO	VAL	69	104	C	CA
HELIX	SHEET	1TMN	65	87	119	122	PRO	TYR	69	122	CA	C
HELIX	SHEET	1TMN	65	87	55	57	ALA	TRP	70	55	CA	CA
HELIX	SHEET	1TMN	65	87	16	25	TYR	ILE	75	20	CA	CA
HELIX	HELIX	1TMN	137	150	65	87	ALA	THR	141	80	CA	CA
HELIX	HELIX	1TMN	137	150	160	180	ASP	GLY	138	173	CA	C
HELIX	HELIX	1TMN	137	150	260	274	THR	LEU	149	271	CA	C
HELIX	SHEET	1TMN	137	150	100	106	LEU	ILE	144	100	CA	CA
HELIX	SHEET	1TMN	137	150	119	122	GLU	MET	143	120	C	CA
HELIX	SHEET	1TMN	137	150	112	115	GLU	TRP	143	115	CA	N
HELIX	HELIX	1TMN	160	180	65	87	VAL	THR	176	80	CA	CA
HELIX	HELIX	1TMN	160	180	137	150	GLY	ASP	173	138	C	CA
HELIX	HELIX	1TMN	160	180	233	246	ALA	SER	163	234	C	CA
HELIX	HELIX	1TMN	160	180	260	274	LEU	ARG	175	260	CA	C
HELIX	HELIX	1TMN	160	180	281	296	GLU	PHE	160	281	C	N
HELIX	HELIX	1TMN	233	246	160	180	SER	ALA	234	163	CA	C
HELIX	HELIX	1TMN	233	246	260	274	SER	ARG	245	260	CA	N
HELIX	HELIX	1TMN	233	246	281	296	ILE	PHE	237	281	CA	CA

Table 4. Sample output from the program Secondary Structure Total Combine for thermolysin (continued).

CROSSING ANGLE	BACKBONE SEPARATION DISTANCE	ATOM CONTACTS	RESIDUE CONTACTS	ATOM CONTACTS PER RESIDUE CONTACTS	CHAIN I.D.	
					1	2
-52.38	5.97	23	6	3.83	E	E
93.67	6.48	16	8	2.00	E	E
162.76	5.89	6	5	1.20	E	E
157.86	5.96	11	6	1.83	E	E
122.78	8.26	1	1	1.00	E	E
-123.02	8.05	9	2	4.50	E	E
71.42	6.17	13	5	2.60	E	E
-52.38	5.97	23	6	3.83	E	E
134.30	4.15	19	10	1.90	E	E
-28.84	7.26	2	2	1.00	E	E
129.15	8.81	2	1	2.00	E	E
168.67	6.46	9	3	3.00	E	E
-47.72	5.51	10	4	2.50	E	E
93.67	6.48	16	8	2.00	E	E
134.30	4.15	19	10	1.90	E	E
-37.17	4.5	9	6	1.50	E	E
-143.08	7.15	17	7	2.43	E	E
-41.37	5.37	14	4	3.50	E	E
-37.17	4.5	9	6	1.50	E	E
131.75	4.69	6	4	1.50	E	E
-22.71	8.11	16	4	4.00	E	E

this program considers only residue-residue interactions between secondary structures. The input for this program is the output from the Combine program.

Helix-Sheet-Residue Pair-Interactions

This program is similar to the previous program, except that rather than consider total secondary structure interactions, this program determines interactions between two helices, between two sheets, between a helix and a sheet, and between a sheet and a helix.

Distribution-Count

For two interacting secondary structures, this program determines the number of residue-residue interactions and atom-atom contacts made for each position relative to the nearest backbone contact residues. The purpose of this program is to be able to profile secondary structure interactions in order to analyze the distribution of contacts made for thermally stable proteins relative to the data base as a whole. This program has the additional feature of being able to ignore artifactual interactions by setting a lower end cut-off for the number of residue-residue interactions.

Distribution-Sum

The output from the previous program serves as the input for this program. This program was run on a concatenated file from the output of the previous program. It gives the number of residue-residue interactions and the average atom-atom contacts/residue-residue interaction for each 30° range of secondary

structure angle contacts. Four separate programs perform these measurements for helix-helix, helix-sheet, sheet-sheet, and sheet-helix interactions.

Residue-Position-Contacts

As in the previous program, interactions are categorized according to angle range and secondary structures involved. This program determines the number of residue-residue contacts and the average number of atom-atom contacts for each residue according to the residues relative position with respect to nearest backbone residues:

Residue-Occurrence-By-Position

These programs determine the frequency of occurrence of each residue at each position relative to the nearest backbone contacts. The programs work on 30° ranges of crossing angles. As in the previous set of programs, the four types of secondary structure interactions are considered separately and the same ranges of backbone contact distances are considered.

Protein-Profile

The total number of residues, total number of atoms, number of polar side chain atoms, number of charged atoms, and number of hydrophobic side chain atoms are computed in this program.

Secondary-Structure-Profile

This program performs the same functions as the previous program, except that rather than compute values for the entire protein, only secondary structures are considered.

Total-Atom-Contacts

This program counts the total number of atom contacts for each residue type.

Secondary-Structure-Atom-Contacts

Same as the previous program, except that only residues and atoms in secondary structures are considered.

Total-Residue-Contacts

This program measures the total number of residue contacts for each residue type.

Secondary-Structure-Residue-Contacts

Same as the previous program, except that only residues in secondary structures are considered.

Total-Residue-Occurrence

The number of occurrences for each residue type are computed.

Secondary-Structure-Residue-Occurrence

The number of occurrences for each residue type in secondary structures are computed.

Total-Contact-Ratio

A set of programs has been devised to measure the ratio of atom-atom contacts made for each residue type per total number of atoms of that residue type as well as the ratio of atom-atom contacts made per total number of residues. This set of programs consists of four individual programs; one program works on programs which measure hydrophobic side chain contacts, another works on programs which measure polar side chain contacts, the third measures charged atom contacts, and the fourth measures the contacts in terms of total residues. For example, Lys is considered to have four hydrophobic atoms per residue and one charged atom. If Lys occurred three times in a protein, the total number of hydrophobic Lys atoms would be 12. The total number of hydrophobic contacts would then be divided by 12. This program profile how many contacts each residue makes for its total number of atoms of that type. This is especially effective when dealing with charged groups. It reduces the bias that Glu, Asp, and Arg have over Lys. The number of atoms which can share charge on each of these residues is two while Lys only has one charged atom.

Secondary-Structure-Contact-Ratio

These programs are identical to the previous programs except that the contacts are between secondary structures and the ratios are for secondary structure atoms or residues.

Angle - Count

This program counts the number of occurrences for each angle range for each type of secondary structure interaction. It only considers secondary structures which have a predetermined number of hydrophobic side chain interactions. In this work, five residue-residue contacts were required before the secondary structures were considered to be interacting.

RESULTS AND DISCUSSION

Protein Interactions

The interaction programs were run on concatenated lists of output for each individual protein. The interactions between residues were then analyzed from three different perspectives: 1)for all interactions in the protein, 2)for interactions between secondary structures, 3)and for interactions between specific secondary structures. Entire protein interactions include interactions between secondary structures, between secondary structures and either loops or turns, between loops, between turns, and between loops and turns. The last category includes helix-helix interactions, helix-sheet interactions, sheet-helix interactions, and sheet-sheet interactions. For some interactions, such as between hydrophobic side chains, there is no distinction between helix-sheet interactions and sheet-helix interactions. For others, such as between polar side chain atoms and backbone amide nitrogen atoms, there is a distinction between helix-sheet and sheet-helix interactions. Finally, for interactions between hydrophobic side chains, preferences in residue-residue interactions were investigated according to the angles at which the secondary structures crossed. While the programs are capable of performing this task on all of the different types of interactions, the other types of interactions were

not studied at this more refined level. Interactions between hydrophobic side chains were initially studied with respect to the separation distance between the backbone atoms in nearest contact. The interactions were investigated as to whether the nearest contact atoms were separated by greater or less than 6.0 Å. However, there were not dramatic differences in the residue-residue interaction preferences and the separation distance approach was subsequently rejected.

Interactions Between Oppositely Charged Groups

The data tables for these interactions are located in Appendix A. All residues are included in this study. This was done to include interactions involving the amino- and carboxy-terminal groups. When all interactions are considered, there appears to be a slight bias for interactions involving Lys over Arg. Glu and Asp occur with nearly equal frequency. For interactions between secondary structures, interactions between Lys residues and Glu residues occur more often than all others. Most of the interactions between oppositely charged groups occur between α -helices. This may reflect a structural role of α -helices and the use of charged groups to strengthen the contact between helices. Interactions between helices and sheets are not common. Between two β -strands, Glu interacts with both Lys and Arg, nearly the same number of times as these same interactions between two α -helices.

Interactions Between Residues of Like Charge

All data for these interactions are in Appendix B. Most of the interactions

between atoms of like charge occur either between two Asp residues or between an Asp and a Glu. This is probably due to some sort of charge-dipole interaction and not really a charge-charge interaction. This will occur when one of the negatively charged groups is involved in a charge-charge interaction with a positively charged groups. This results in the charge distribution lying primarily on one of the atoms, allowing the other atom to interact with a charged group. The programs are unable to make this distinction. The number of interactions between these residues drops dramatically when going from the entire protein to interactions between secondary structures. The high number of interactions on the whole protein level may result from the high cut-off distance (5 Å) and the clustering of charged residues near active sites. Since active sites often involve residues in loops, these interactions do not show up when secondary structures are considered.

Interactions Between Charged Atoms and Polar Backbone Atoms

The data for interactions between charged atoms and polar backbone atoms are located in Appendix C. As would be expected, the negatively charged residues interact much more frequently with amide backbone nitrogen atoms than do positively charged residues. Conversely, positively charged residues interact more frequently with carbonyl backbone oxygen atoms than negatively charged residues, although the preference is not as pronounced. However, the interactions between secondary structures are greatly reduced when compared to total protein

interactions. It is noteworthy that, for interactions between secondary structures, all of the interactions involving the amide nitrogen of Pro occur between Pro and Arg residues.

Charged Atom - Polar Side-Chain Atom Interactions

The data for this section are in Appendix D. The high number of Arg-Glu and Arg-Asp interactions are probably not an accurate reflection of charge-dipole interactions. The ϵ nitrogen atom is considered polar in this work. These results suggest that this may not be an accurate assignment. The resonance stabilization of the guanido group can result in the ϵ nitrogen atom carrying a positive charge and this would appear to be the case. The most interactions occur between Asp and Ser residues. Interactions between charged atoms and polar side-chain atoms do not play a significant role in interactions between secondary structures. Lys, with a total of 12 interactions, makes a surprisingly small contribution. Of these interactions, most of them take place between β -strands. Most inter-helical interactions occur between either Asp and Tyr or Glu and His. This raises the question of the importance of interactions between charged and polar side-chain atoms. Perhaps more importantly are the positions of these groups in their respective secondary structures and how involved the ends of helices are involved in these interactions.

Polar Side-Chain Atom - Polar Side-Chain Atom Interactions

Tables for the interactions between polar side-chain atoms are in Appendix E. On the entire protein level, the largest number of interactions take place between two Asn residues. The nitrogen side chain atom of Trp does not interact with itself and there is only one interaction between this atom and the polar His atoms. The aromatic side-chains in general exhibit a marked preference for the smaller straight chain polar side-chains. Only interactions between His residues occurs in any significant number. This is perhaps indicative of the lack of importance of these hydrogen bonds in the overall stabilization of the protein.

It is somewhat surprising that there are more interactions between two His residues than any other polar side-chain atom contact. Of the 16 His-His interactions, 10 occur between two β -sheets and six occur between two α -helices. There were no interactions between an α -helix and a β -sheet. While Asn residues interacted with themselves 56 times in the entire protein, only two of those contacts occurred between secondary structures and both of those occurred between helices. There are only a total of 26 interactions between α -helices and β -sheets. This is roughly one interaction for every three proteins studied. Clearly, these interactions are not of critical importance between helices and sheets. Thr makes more contacts with other polar side chain residues than any other residue between two β -strands. The preferred interactions for Thr are between two Thr residues and between Thr and Ser residues.

Polar Side-Chain Atom - Polar Backbone Atom Interactions

The data tables for this section are located in Appendix F. A possible contribution to stability would be the ability of polar side-chain atoms to form hydrogen bonds with backbone atoms and thus stabilize secondary structures. While there are a large number of contacts made in the entire protein, there are surprisingly few between secondary structures. Interactions occur more frequently between polar side-chain atoms and carbonyl oxygen atoms than amide nitrogen atoms. This probably reflects the accessibility of the oxygen atom, which protrudes somewhat from the backbone. While these interactions may be stabilizing, apparently the unfavorable energy required to position the side chains next to the backbone overcomes the favorable energy contribution.

Backbone Atom - Backbone Atom Interactions

This work does not distinguish between hydrogen bonded backbone atoms and other contacts. Not surprisingly, most of the interactions between secondary structures occur between two β -strands. This is due to the inability of the programs to disregard interacting strands which are part of the same sheet.

There are differences in the interactions which occur for the entire protein and those which occur between secondary structures. For example, there are a total of 55 Ala-Ile backbone interactions and 104 Ala-Leu interactions. Between secondary structures, there are 38 Ala-Ile interactions and 28 Ala-Leu interactions.

It is curious that the number of Ala-Leu interactions drops so dramatically. Between helices, the highest number of interactions is between two Gly residues. This is likely to be caused by a combination of Gly residues occurring near the nearest backbone contact point and the lack of side-chain steric hinderance.

There are very few backbone interactions between α -helices and β -sheets. This probably reflects the importance of side-chain packing when these two secondary structures interact. While it would appear feasible that helices and sheets would form backbone hydrogen bonds in β - α - β motifs, this does not appear to occur significantly.

The backbone interactions which occur between β -strands seems to hold the most information. The high number of Val-Val interactions suggests that these residues are capable of residing next to each other in adjacent β -strands. The lack of interactions may be useful in predicting which residues reside next to each other on adjacent β -strands. There are no interactions between Trp and either Cys, Asn, Lys, or Phe. These types of preferences may help in the alignment of β -strands to form β -sheets.

Backbone Atom - Hydrophobic Side-Chain Atom Interactions

Interactions between backbone atoms and hydrophobic side-chain atoms are in Appendix G. The drop in the number of interactions from the entire protein to interactions between secondary structures is not as pronounced for backbone-hydrophobic side chain contacts as most of the other interactions. This may reflect

the level of packing between secondary structures related to the protein in general. One might anticipate that the number of contacts would be higher between β -strands than between α -helices on the basis of proximity of the β -strands. However, the numbers are surprisingly equal.

Hydrophobic Side-Chain - Hydrophobic Side-Chain Interactions

The data tables for this section are in Appendix H. When looking at interactions between entire proteins, it is not easy to distinguish preferential interactions between residues. Clearly, there is a strong preference for Leu residues to interact with each other. This bias is observed at nearly all levels of investigation.

At the level of interactions between secondary structures, without regard to specific secondary structure type, some interactions become conspicuous by their absence. The hydrophobic moiety of Asn residues are never observed to contact each other in any secondary structures. This may prove valuable in structure prediction or the designing of proteins.

At the level of interactions between specific secondary structures preferences become increasingly apparent. A number of different types of interactions are absent. For example, between helices, the hydrophobic portion of the Asn side-chain does not interact with Asn, Cys, or Glu hydrophobic side chain atoms. Gln residues are not observed to interact with Asp, Cys, Gln, Pro, or Thr residues. Nearly all residues interact more frequently with Leu residues

than all others. Potential disulfide bonds are less prevalent between two interacting helices than for either helix-sheet or sheet-sheet interactions.

Interactions between helices and sheets also exhibit preferences. While Phe residues were shown to interact frequently between two helices, the number is much reduced for interactions involving an α -helix and a β -sheet. When the interaction involves Phe residues, both of which belong to β -sheets, the interactions are nearly as frequent as those between helices. For Leu and Ile residues belonging to β -sheets, both are nearly as likely to interact with all helical residues.

For interactions between β -strands, interactions between two Val residues occur 152 times while interactions between two Ala residues occur only six times. While Ile is often considered to be a preferred residue for β -sheet interactions, most residues occur more frequently with Leu. This tendency is more dramatic for residues with branched side-chains.

Hydrophobic Side-Chain Interactions by Angle Ranges

All data for this section are in Appendix I. At this level, preferential interactions between amino acids become more prevalent. Interactions between pairs of residues are observed for some crossing angle ranges, while they are absent at others. Obviously, preferences for interactions between residue pairs are observed depending upon whether the secondary structures involved are two α -helices, two β -sheets, or an α -helix and a β -sheet. A noteworthy observation

are angle ranges where aromatic groups tend to interact and angles where disulfide bonds occur.

Helix-Helix Interactions

There are few outstanding interactions between helices in the low positive angle range. As with all inter-helical contacts, Leu-Leu interactions tend to dominate, most likely due to the ability of the branched side chains to interdigitate. These results reinforce the dogma that Ile residues are not significant contributors to interactions between helices. Presumably, the branching of the side chain at the β -carbon and the two hydrocarbon extension on one side of this branch bias against Ile in α -helices. Clearly, branching at the β -carbon alone is not enough to result in this observation as Val is also branched at the β -carbon and plays a significant role in certain angle ranges. The fidelity of the programs employed here does not shed light as to why this bias should exist.

There are only two angle ranges at which potential disulfide bonds exist. There are four potential interactions in the angle range of 150° and 180° and two potential interactions in the angle range of -90° and -120° . It is noted that with the cut-off distance for interactions set at $0.4 \text{ \AA}$ greater than the sum of the van der Waals radii, two Cys residues which are not involved in a disulfide bond could be interpreted as being involved in a disulfide interaction.

Interactions between Leu residues are particularly dominant in the angle range $0^\circ - 90^\circ$. In this angle range, there are not many interactions between helices, a result which exemplifies the preference for helices to be antiparallel. In

the angle range 90° to 120° , Leu-Val interactions are almost as prevalent as Leu-Leu interactions. Also, the number of Phe-Phe interactions is high. In fact most of the interactions between Phe residues occur when α -helices are perpendicular to each other. This preference is strong enough that it may be predictive for how α -helices align themselves when Phe residues are present. The other aromatic residues do not display such marked preferences. This raises the question as to whether it is difficult to align helices within certain angle ranges when bulky aromatics are present at certain positions. There is not a marked preference for Phe residues at various positions for the perpendicular crossing angles. In fact, Phe occurs at or near the nearest contact backbone residue a number of times. Perhaps aromatic side-chains are better able to interdigitate at these angle ranges.

Between 90° and 120° , there are 56 Leu-Leu interactions, 8 Phe-Phe interactions and 15 Val-Val interactions. For the angle range 120° - 150° , there are 6 Leu-Leu interactions, 0 Phe-Phe interactions, and 14 Val-Val interactions. When combinations of residues are considered, the ability to accurately predict the crossing angles of helices may be increased.

Helix-Sheet

Patterns of interactions between helices and sheets are more difficult to discern than interactions between pairs of helices. Even the angle ranges of disulfide bonds are more evenly distributed. There is a slight preference for disulfide to occur between the angles 90° and 150° , where five disulfides are observed.

Preferential interactions between helices and individual strands located at specific positions within the β -sheet may be distinguishable. However, until larger databases are investigated, the preferences probably will not be meaningful. For an accurate assessment of interactions involving β -sheets, interactions involving individual strands and the location of these strands in the β -sheet must be considered.

Sheet-Sheet

Interactions between Ala residues are conspicuous by their absence. Seldom do Ala residue interact with each other at any angle range. This may be useful when aligning two β -strands. However, Ala does interact with branched side-chain residues in a number of instances. Phe residues, analogously to interactions between α -helices, makes a number of interactions when two β -strands cross each other nearly perpendicularly. The predominant interactions appear to be between residues with branched side chains. Val tends to be more involved in interactions both with itself and with other branched hydrophobic groups at angles which are more nearly parallel or antiparallel. At angles in which the two strands are more nearly perpendicular, the interactions between the other branched residues become increasingly favorable.

Ala Interactions in Helical Pairs with Crossing Angles Between -150° and -180°

The data tables for this section are in Appendix J. The angle range of -150° to -180° was chosen so that a well defined motif, the four-helix bundle, could be

studied. The data presented in appendix J reflect the final most complete analysis of interactions. It is obvious that the boundaries of meaningful data have been reached. These tables represent Ala residues at the various positions relative to the nearest backbone contact residues. All of the interactions involve hydrophobic side-chain atoms in pairs of helices which cross each other at angles which range from -150° and -180° . The tables list not only which residues interact with Ala, but the positions of both residues in their respective helices. For Ala at positions in which no interactions were recorded, the tables are omitted. These programs can be performed on any residue for any angle range between any two secondary structures. These data have the potential to be extremely valuable in assessing which residues will interact with each other at different positions. This program is the logical end which can be used to assess the secondary structure packing aspect of protein structure prediction. Additionally, these data should serve useful in designing proteins, where it would be advantageous to know preferential interactions for residues at certain positions and the residues which interact with them.

Ala is only involved in three interactions when it resides on the amino-terminal portion of the helix. While it is logical to assume that Ala residues at the nearest backbone contact position would interact with other residues at their nearest backbone contact positions, there is a preference for Ala to interact with residues at the +3 and +4 positions. It is not immediately obvious why this preference exists, as it is not obvious why Ala is not more involved at the negative

positions. The branched hydrophobic residues at positions +3 and +4 seem capable of interacting with Ala at position 0.

Ala has a preference for interactions when it is located at multiples of three and four from the 0 position. This may reflect a preference for being located in the hydrophobic region of the packing face or may merely reflect that its small size precludes interactions unless it is more directly oriented toward the other helix. The residues interacting with Ala also appear to be oriented toward the hydrophobic packing face of the interacting helices.

At present, the number of helices which fall into the -150° to -180° angle range limit the usefulness of this program.

Interactions by Position

These programs measure the number of residue contacts made and the average number of atom contacts for each position for each angle range.

Backbone-Backbone Interactions

The data table which pertain to this section are in Appendix K. There are no interactions between backbone atoms for helix-sheet interactions for negative crossing angles. For interactions between two β -strands, the greater number of interactions in the angle range of -180° to -150° as compared with the angle range of 0° to 30° reflects the preference of parallel β -sheets to align in this manner. This is caused by the right handed twist of the β -sheets as the individual strands pack. This preference is also observed in antiparallel β -sheets where the angle

range of 150° to 180° is preferred over the angle range of 0° to -30° .

Backbone-Hydrophobic Side-chain Interactions

Not surprisingly, as the angles between helices become closer to parallel or antiparallel, hydrophobic side chains contact backbone atoms at positions further removed from the nearest backbone contact atoms. Most of the helical backbone atoms which are contacted by hydrophobic side chains occur in the 150° - 180° angle range, which reflects the angle range for β - α - β motifs. The number of helical side chains contacting sheet backbone atoms is also high for this angle range. Most of the interactions are toward the amino-terminal end of the β -strands involved. It is not intuitively obvious why this preference should occur. For interactions between β -strands, the interactions reflect the preferred parallel or antiparallel alignment of the strands.

Charged Atom-Polar Backbone Atom

There were no interactions between charged atoms and amide nitrogen backbone atoms for any helical-sheet interactions. It should be pointed out that there were a minimum number of six hydrophobic side chain contacts between secondary structures for these interactions to be counted in this portion of the work. This accounts for the discrepancy between these results and the residue preferences which show hydrophobic side chain backbone atom contact. Similarly, charged helical groups did not contact amide nitrogen backbone atoms of β -sheets. The interactions between β -strands are somewhat more numerous.

Charged Atom - Polar Side-Chain Interactions

Most of the interactions occur between either pairs of helices or pairs of β -strands. While the number of contacts is not large, it is noted that for interactions between β -strands, the charged residue is often at the point of nearest backbone contact.

Hydrophobic Side-Chain Atom Interactions

Interactions between α -helices display a periodicity of interaction which roughly reflects the 3.6 residues/turn nature of the helices. Helices which cross at more perpendicular angles tend to have a narrower distribution of contacts with the contacts occurring closer to the points of nearest backbone contact. Helices which are more parallel or antiparallel in nature, such as four-helix bundles tend to have a larger distribution of contacts.

Charged Atom Interactions

There is no strong position preference for any of the angle ranges for inter-helical interactions. There does not seem to be a bias against charged residues at the nearest backbone contact position. While it might be expected that this position could be dominated by hydrophobic residues which could form a very nonpolar interface, charged residues still are found to reside at these positions. There are too few interactions between helices and sheets to be of any note. Interactions between β -strands show that there is a clear bias for interactions

between antiparallel strands as compared to interactions between parallel strands. However, this may merely reflect a the greater number of antiparallel β -strands.

Polar Side-Chain - Polar Backbone Interactions

There are few interactions involving nitrogen backbone atoms for any of the secondary structure pairs studied. Most of the interactions involve pairs of β -strands. For interactions involving a β -sheet and an α -helix, all of the sheet side chain residues were located at the point of nearest backbone contact. Antiparallel β -strands exhibit the most contacts and the widest range of distribution of all sheet-sheet contacts.

Polar Side-Chain Interactions

There is a slight periodicity to interactions between helical polar side-chain atoms. There are too few interactions to allow decisive conclusions. As with nearly all other interactions, there were fewer occurrences between helices than sheets. Most of the contacts between β -strands occur at positions which immediately flank the nearest contact residues for antiparallel β -sheets.

Preferences by Position

All data tables for this section are in Appendix L. The cut-offs for these interactions are 12 residues on either side of the closest backbone residues. Certainly, there are residues which are further distant which interact and these residues are not accounted for. These data tables list the number of occurrences

of each amino acid at each position for each crossing angle and give a good overall perspective on the general types of residues which are found at different positions.

Helix-Helix

It is particularly interesting to track the frequencies of occurrence of the residues Ala and Leu, as they constitute such a large percentage of α -helices. In nearly all of the angle ranges, there is a periodicity to the occurrences of Leu. The period of repeat tends to be between three and four. This most likely reflects the amphiphilicity which is so often characteristic of α -helices. What is interesting to note is that for a number of angle ranges, Leu occurs more often than all other residues combined. While Leu is often not a preferred residue for the nearest contact residue, it is often found to flank the nearest contact residue. This may suggest that Leu is utilized to maximize the number of contacts near the backbone contacts.

The occurrences of Ala residues at the nearest backbone contact position is readily apparent, in agreement with the work of others(27). However, in contrast to their work, Gly is seldom found at this position. As was suggested in the initial studies, Ala's presence may allow the backbones to come into nearer contact and thus increase the number of contacts between the helices.

The periodicity of Val residues and the preferential occurrences at certain positions roughly parallels that of Leu.

The periodicity of occurrence of charged and polar residues is not nearly as

pronounced as it is for hydrophobic residues. Additionally, there is not a clear preference for these residues at positions which are not occupied by hydrophobic residues.

It seems feasible that large aromatic groups would be found in outlying positions. The rationale for this is that they would make contacts at distances which would be more difficult for smaller residues. Additionally, the placement of these relatively rigid side chains in crowded regions near the closest backbone contact residues would seemingly be problematic. However, there is not a marked preference for the aromatic residues for outlying regions and they do not display periodicities of occurrence which could be useful in characterizing helix-helix interactions.

Helix-Sheet Interactions

Useful information is sometimes conspicuous by the absence of interactions. There are no occurrences of helix-sheet interactions in the 30° to 60° range. Additionally, the periodicity of occurrence of the hydrophobic residues is not so readily apparent for α -helices interacting with β -sheets.

The number of occurrences of Ala residues in the angle ranges 150° to 180° and 0° to -30° is noteworthy. The number of occurrences of helices and sheets interacting in the angle range of 150° to 180° is understandable due to the antiparallel alignment of helices and sheets in α/β barrels and α/β open twisted sheets. The high frequency of occurrence of Ala residues in these interactions may be useful in predicting these super-secondary structures.

Sheet-Sheet Interactions

There are not the marked periodicities that one might expect for β -sheets. Amphiphilic β -sheets should exhibit a periodicity of 2. The lack of periodicity may be due to the less amphiphilic nature of β -sheets with respect to α -helices. This is caused by a preference for helices to reside near the surface and for sheets to reside more often in the interior. It is also possible that the packing of β -strands may position the backbones such that the closest contact may lie nearly the same distance between two residues. Since the program returns only one value for the nearest backbone contact, this would not be observable at present.

Charged groups are often located near, and sometimes at, the point of closest backbone contact. Clearly, β -sheets do not tend to contain many residues and there is a clear bias for residues to reside near the point of nearest contact. The patterns of position preference are more difficult for sheet-sheet interactions than for the other secondary structure interactions. This may explain the difficulty in predicting how β -sheets pack. A more sensitive program would appear to be necessary. A program which looks at interactions between three residues or interactions between three secondary structures could possibly help to shed insight on β -sheet packing. Additionally, if strand position with regard to the sheet as a whole were taken into account, this problem could possibly also be circumvented.

Contact Ratios

All tables dealing with contact ratios are in appendix M. For most interactions, four different contact ratios were investigated. These generally were divided into two contact ratios for interactions involving the entire protein and two contact ratios for interactions between secondary structures. For example, when studying interactions between polar side-chain atoms on the whole protein scale, the number of contacts made by each residue type were divided by the number of occurrences of that residue type. Additionally, the total number of polar side-chain contacts was divided by the total number of polar residues. Then, the number of polar interactions were divided by the total number of polar atoms for each residue type and the total polar contacts were divided by the total number of polar atoms. In this study, the side chain of Asn was considered to have two polar atoms. Next, the polar side-chain interactions between secondary structures for each individual polar residue were divided by the number of occurrences of that residue. Again, the total number of contacts were divided by the total number of polar residues from secondary structures. Finally, for each residue type, the number of contacts were divided by the total number of polar atoms of that residue type which resided in secondary structures. The outputs from all proteins were joined for each contact ratio and listed in descending order with regard to the ratio involving total interactions. The objective of this approach was to look at a number of possible combinations to determine if thermally stable proteins were clearly distinguishable from other proteins.

The heat stable proteins thermolysin and T4 lysozyme do not clearly distinguish themselves from other proteins in any given contact ratio. There are several instances where they appear to make higher ratios of contacts. This lack of a clear distinction between heat stable proteins and proteins in general suggest that protein stability is a result of a combination of a number of favorable factors and no one type of interaction is critical for stability.

While it would appear logical that stable proteins would exhibit a very high ratio of hydrophobic side-chain contacts, this is not the case. Thermolysin and T4 lysozyme are above average with respect to the number of hydrophobic side-chain interactions between secondary structures, but not glaringly so. When the entire protein is considered, both of these proteins become decidedly average.

Heat stable proteins appear to make more favorable contacts than other proteins in interactions involving charged groups with polar side-chain atoms. Both thermolysin and T4 lysozyme involve a relatively high percentage of their oppositely charged residues in electrostatic interactions, at least for interactions involving secondary structures. For thermolysin, there is a dramatic lowering of its ranking when the oppositely charged atom interactions are considered for the whole protein.

Thermolysin, in particular appears to have a very high ratio of favorable contacts involving charged residues. It is one of the highest proteins for contact ratios for charged atom polar side-chain atom contacts with respect to the entire protein and interactions between secondary structures. Additionally, thermolysin

has a high ratio of contacts involving atoms of like charge. While at first glance, this would appear to be energetically unfavorable, it will be discussed in the thermolysin section that this is due to negatively charged atoms interacting with the same Ca ions.

Thermolysin

The raw data gathered in this work is applied to the analysis of the thermally stable endopeptidase thermolysin. Thermolysin is particularly interesting to study as it contains no disulfide bonds which could contribute to stability. At the present stage of development, it is necessary for the user to analyze data from the programs and draw conclusions.

Three different characteristics of thermolysin will be discussed. It will be suggested that the architecture of secondary structures plays a significant role in thermolysin's stability. It will also be suggested that metal ions contribute to the stabilization of secondary structures. Finally, it will be shown that thermolysin stabilizes its amino- and carboxy-termini. It will be argued that these features can be employed in the de novo design of proteins.

Interactions Between Secondary Structures

α -helices have long been considered to behave as semi-rigid structural units. In this sense, they can serve as building blocks for proteins. The total number of hydrophobic side-chain atom contacts between secondary structures was investigated. Helices were studied which made ten or more hydrophobic side-

chain atom contacts with each other. For thermolysin, it was observed that there were a number of helices which interacted with each other. More specifically, triads of interacting helices were observed, in which each helix participated in ten or more atom contacts with both other helices. Out of 67 proteins investigated, only four contained triads of interacting helices. The other three proteins were cytochrome p450, citrate synthase, and phage T4 lysozyme. Interestingly, T4 lysozyme is also thermally stable. Thermolysin has three helical triads by these standards. If the requirement of ten hydrophobic side chain atom contacts is relaxed to nine contacts, thermolysin has four helical triads. Only citrate synthase has more. Clearly, helical triads are not a guarantee of thermal stability, but it does appear as though they may play an important role, at least for some proteins.

Two α -helices are critically involved in helical triads. These helices consist of residues 160-180 and residues 281-296. If the softer nine hydrophobic side-chain atom contact standard is employed, both helix 160-180 and helix 281-296 are involved in three helical triads. Helix 160-180 projects nearly through the middle of thermolysin and appears to form the core of the molecule. These helices are common to two helical triads and each is involved in a triad which is separate from the other helix.

One of the helical triads is particularly interesting in the manner that the three helices interact with each other. This triad consists of helix 160-180, helix 65-87, and helix 137-150. While the rest of the molecule is predominantly helical, this triad interacts with most of the β -sheet loop structure and may need to provide

a strong structural framework. The angle between helices 65-87 and 160-180 is 94° . The angle between helices 137-150 and 160-180 is 134° . The angle between helices 65-87 and 137-150 is -52° . Disregarding the direction factor in the determination of angles, the angles become 94° , 52° , and 45° . This is very close to the optimal angles used in building construction, where a post and beam form a 90° angle and the supporting cross brace forms 45° angles with both the post and beam. Perhaps theories of Newtonian physics can be applied to protein design and concepts such as moment of inertia between secondary structures will be important. Additionally, the Zn ion is coordinated with a His residue from each of the helices 137-150 and 160-180. Two Glu residues from helix 137-150 are also within 5.0° . The Zn ion may serve to form an electrostatic bridge between these helices. These contacts may serve to provide a more stable active site, which may be difficult to accomplish under the high temperature conditions native to this molecule. Also, an Asp residue from helix 137-150 and a Glu residue from helix 160-180 both interact with the same Ca ion. The four Ca ions in thermolysin form a total of nine contacts with charged groups, six contacts with polar backbone atoms, and one contact with a polar side-chain atom.

Thermolysin makes several interactions with its terminal residues. The carboxy-terminal Lys residue forms a charge-dipole interaction with a Ser residue from helix 281-296. Additionally, the backbone carboxyl group of this Lys residue interacts with a guanido group from an Arg residue in helix 281-296. The amino-terminal amine group of residue Ile 1 forms a charge-dipole group with the side

chain of Gln 31. Additionally, the side chain of this Ile residue is involved in 11 hydrophobic side-chain contacts.

The α -helices of the thermally stable phage T4 lysozyme form two helical triads, if the criterion of nine hydrophobic side-chain atom contacts are employed. Helices 93-106, 3-11, and 60-80 form one of the triads while helices 93-106, 143-155, and 126-134 form the other. Helix 93-106 appears to serve a similar role as helix 160-180 does in thermolysin in that it forms the core of the molecule. Charged residues at or near the ends of helices form electrostatic salt-bridges between two helices from the individual triads. Asp 10 contacts both Arg 145 and Arg 148 while Glu 11 contacts Arg 145. As helices 3-11 and 143-155 do not meet the criterion for hydrophobic side-chain contacts, these electrostatic interactions appear to tether their respective triads.

Citrate synthase has the largest number of helical triads. Possible explanations as to why it is not listed as thermally stable may be the fact that it is a dimer and it does not stabilize the ends of its chains. Additional factors, such as an unfavorable hydrophobic-hydrophilic distribution or mechanical stress on loops or turns may be involved. However the programs used in this work would not provide insight into these factors.

SUMMARY

The system designed in this work accomplished its objectives as follows:

- 1) It is capable of detecting a variety of interactions between residues, 2) It is capable of determine which secondary structures are involved in these interactions, 3) The analysis of crystal structures with a Brookhaven database format is automated, 4) The results of this work can be incorporated into programs which predict protein structure or programs which aid in protien design.

The programs developed here are not sufficient to predict tertiary structure or even distinguish thermally stable proteins from their less stable counterparts. At this stage in the development, these programs yield large amount of data which can then be analyzed to determine factors which may be of critical importance to protein stability. From the analysis of these data, new programs can be designed to incorporate the worthwhile findings in an effort to develop a system which will be capable of predicting tertiary structure.

The programs presented here do not address interactions between specific atoms. Eventually, these interactions as well as the dihedral angles of the residues should be incorporated into later stages of development.

Admittedly, these programs are not complete and far from perfect. There was considerable subjective decision-making which went into the assignment of values within the programs. Many of the values could be argued against and

probably correctly so. In retrospect, the assignment of the ϵ nitrogen atom of Arg's side-chain was probably incorrect. The number of interactions with negatively charged atoms suggest that this may be more than an artifact of the interaction between the negative atoms and the terminal amine groups of Arg. Also, the guanido carbon, which was analyzed as an hydrophobic atom is certainly capable of carrying a charge through resonance stabilization. The cut-off distances which were employed for hydrophobic contact, charge-dipole contact, dipole-dipole contact, and charge-charge contact were subjective and analysis using a number of values to determine the most accurate values would be valuable. Adopting a graduated scale for hydrophobic contacts could reflect more realistic van der Waals values. It is understood that the assignment of a single value for all interactions is a gross simplification and ignores the local environment. This becomes especially problematic when dealing with charged groups where the local environment has a profound effect on the dielectric constant.

An accurate determination of the axes of the secondary structures involved in interactions between secondary structures is a future goal of this work. This would allow the determination of nearest contact of the secondary structure axes. The crossing points could then be used to measure the distance of residues along the axis which would be a more accurate assignment of the relative positions of residues. Additionally, a method to incorporate the rotational positions of residues with respect to the orientation of the secondary structures would be useful.

Many of the data tables do not contain enough information to be

immediately valuable. However, the goal was to design a system which would become increasingly worthwhile as the size of the database increases. To this end, these programs will become a more accurate reflection of the interactions which take place between residues. This will become increasingly useful when applied to the design of de novo proteins.

In contrast to the earlier work of others, there do seem to be preferential interactions between residues (58). This becomes more apparent as contacts are analyzed with respect to the crossing angles of secondary structures. Preferences between the same residues occasionally vary from one angle range to the next. This information will hopefully be applicable in the prediction of protein structure and the design of novel proteins.

The results obtained in this work suggest that the next phase of development should be the study of the interactions between three interacting residues and three interacting secondary structures. These programs would then be able to include the effect residues in the same secondary structure exerted upon each other. Of course, a larger database will need to be analyzed for the results to be meaningful, but the analysis of triads of interacting residues from the perspective of crossing angle and relative backbone position may be specific enough to predict structure and design proteins. The approach of studying the interactions between triads of secondary structures seems to hold great promise and an automated system for accomplishing this is neither difficult nor unrealistic. The study of secondary structure triads would improve the ability to predict the

packing of structures such as β - α - β motifs which function as the building blocks for α/β barrels and α/β open-twisted sheets.

The speed and ease of application of these programs make analysis of proteins an efficient process. This proved to be valuable in the study of thermolysin. While it required interpretation, the raw data expedited the recognition of helical triads. These triads appear to be fundamental building blocks contributing to the stability of thermolysin. The occurrence of these helical triads in the thermally stable protein phage T4 lysozyme further underlie their significance. The ability of thermolysin to form favorable interactions with its termini coupled with the electrostatic bridging of secondary structures through mutual interactions with ions is also noteworthy.

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APPENDICES

APPENDIX A

Table 6: Total number of residue-residue interactions and average atom contacts for interactions between secondary structures for oppositely charged atoms.

[illegible]

Table 7: Number of residue-residue interactions and average atom contacts for interactions between oppositely charged atoms. Interactions are between pairs of α -helices.

[illegible]

Table 8: Number of residue-residue interactions and average atom contacts for interactions between oppositely charged atoms. Interactions are between α -helices and β -sheets.

[illegible]

Table 9: Number of residue-residue interactions and average atom contacts for interactions between oppositely charged atoms. Interactions are between β -sheets and α -helices.

[illegible]

APPENDIX B

Table 10: Number of residue-residue interactions and average atom contacts for interactions between oppositely charged atoms. Interactions are between pairs of β -sheets.

[illegible]

1. The first step is to identify the problem. This involves understanding the current situation and what needs to be achieved.

Table 13: Number of residue-residue interactions and average atom contacts for interactions between atoms of like charge. Interactions are between pairs of α -helices.

[illegible]

Table 14: Number of residue-residue interactions and average atom contacts for interactions between atoms of like charge. Interactions are between α -helices and β -sheets.

[illegible]

Table 15: Number of residue-residue interactions and average atom contacts for interactions between atoms of like charge. Interactions are between β -sheets and α -helices.

[illegible]

APPENDIX C

Table 17: Total number of residue-residue interactions and average atom contacts for interactions between charged atoms and backbone carbonyl atoms.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	1	0	1	0	0	1	2	0	0	0	0	0	0	0	1
ALA	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
ARG	28	13	19	20	8	8	12	31	15	6	28	14	7	13	23	23	19	4	12	13
ARG	1.2	1.0	1.2	1.1	1.0	1.2	1.2	1.2	1.1	1.2	1.2	1.2	1.3	1.4	1.2	1.1	1.1	1.2	1.1	1.2
ASN	0	0	0	0	0	0	0	0	0	3	1	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	14	8	21	9	10	18	18	29	4	11	10	41	4	9	2	28	36	4	15	15
ASP	1.4	1.2	1.1	1.2	1.1	1.3	1.2	1.2	1.0	1.2	1.1	1.5	1.2	1.2	1.0	1.2	1.3	1.0	1.1	1.2
CYS	0	0	0	0	0	0	0	0	0	0	0	2	0	0	1	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
GLN	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLN	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	5	4	10	8	1	4	2	14	5	3	3	8	2	7	2	5	3	2	4	6
GLU	1.0	1.0	1.1	1.2	1.0	1.0	1.0	1.2	1.2	1.0	1.0	1.3	1.0	1.3	1.0	1.0	1.3	1.0	1.0	1.0
GLY	0	2	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ILE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LEU	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
LEU	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LYS	26	7	22	18	1	10	11	23	5	8	19	16	2	8	4	24	18	1	6	15
LYS	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.5	1.0	1.2	1.0	1.0	1.0	1.0	1.0
MET	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0
PHE	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
PHE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PRO	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PRO	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	1	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
THR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0
VAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

[illegible][illegible]

ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
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[illegible]

Table 21: Number of residue-residue interactions and average atom contacts for interactions between charged atoms and backbone carbonyl oxygen atoms. Interactions are between β -sheets and α -helices.

[illegible]

Table 22: Number of residue-residue interactions and average atom contacts for interactions between charged atoms and backbone carbonyl oxygen atoms. Interactions are between pairs of β -sheets.

[illegible]

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	1	0	1	0	0	1	2	0	0	0	0	0	0	0	1
ALA	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
ARG	28	13	19	20	8	8	12	31	15	6	26	14	7	13	23	23	19	4	12	13
ARG	1.2	1.0	1.2	1.1	1.0	1.2	1.2	1.2	1.1	1.2	1.2	1.2	1.3	1.4	1.2	1.1	1.1	1.2	1.1	1.2
ASN	0	0	0	0	0	0	0	0	0	3	1	0	-0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	14	9	21	9	10	18	18	29	4	11	10	41	4	9	2	26	36	4	15	15
ASP	1.4	1.2	1.1	1.2	1.1	1.3	1.2	1.2	1.0	1.2	1.1	1.5	1.2	1.2	1.0	1.2	1.3	1.0	1.1	1.2
CYS	0	0	0	0	0	0	0	0	0	0	0	2	0	0	1	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
GLN	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLN	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	5	4	10	6	1	4	2	14	5	3	3	6	2	7	2	5	3	2	4	6
GLU	1.0	1.0	1.1	1.2	1.0	1.0	1.0	1.2	1.2	1.0	1.0	1.3	1.0	1.3	1.0	1.0	1.3	1.0	1.0	1.0
GLY	0	2	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ILE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LEU	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
LEU	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LYS	26	7	22	16	1	10	11	23	5	8	19	16	2	8	4	24	18	1	6	15
LYS	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.5	1.0	1.2	1.0	1.0	1.0	1.0	1.0
MET	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0
PHE	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
PHE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PRO	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PRO	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	1	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
THR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	0	0	-0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0
VAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 24: Total number of residue-residue interactions and average atom contacts for interactions between secondary structures for charged atoms and backbone nitrogen atoms.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
ALA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
ARG	4	1	0	4	1	4	2	5	1	1	1	2	2	2	8	5	5	1	3	2
ARG	1.0	1.0	0.0	1.0	1.0	1.2	1.0	1.0	1.0	1.0	1.0	1.5	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	62	27	68	46	18	33	36	116	18	21	23	65	8	23	30	108	87	15	18	32
ASP	1.0	1.0	1.1	1.1	1.2	1.1	1.1	1.1	1.0	1.2	1.0	1.0	1.0	1.0	1.0	1.1	1.1	1.0	1.0	1.1
CYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	18	7	23	17	1	5	16	28	8	5	7	14	2	9	15	27	20	3	4	6
GLU	1.1	1.0	1.1	1.1	1.0	1.0	1.4	1.1	1.1	1.0	1.0	1.0	1.0	1.1	1.0	1.2	1.0	1.0	1.0	1.0
GLY	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ILE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LEU	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
LEU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LYS	1	1	0	3	0	0	0	3	0	1	0	2	0	0	0	1	0	1	0	0
LYS	1.0	1.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0
MET	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
PHE	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PHE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PRO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
VAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 25: Number of residue-residue interactions and average atom contacts for interactions between charged atoms and backbone nitrogen atoms. Interactions are between pairs of α -helices.

[illegible]

Table 27: Number of residue-residue interactions and average atom contacts for interactions between charged atoms and backbone nitrogen atoms. Interactions are between β -sheets and α -helices.

[illegible]

Table 28: Number of residue-residue interactions and average atom contacts for interactions between charged atoms and backbone nitrogen atoms. Interactions are between pairs of β -sheets.

[illegible]

APPENDIX D

Table 30: Total number of interactions and average atom contacts for interactions between secondary structures for charged atoms and polar side-chain atoms.

	ARG	ASN	GLN	HIS	SER	THR	TRP	TYR
ALA	0	0	0	0	0	0	0	0
ALA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARG	1	9	8	4	9	2	4	5
ARG	1.0	1.4	1.2	1.0	1.2	1.0	1.0	1.0
ASN	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	9	15	7	13	5	11	7	24
ASP	1.3	1.3	1.6	1.5	1.4	1.3	1.1	1.2
CYS	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	10	10	7	13	11	3	2	8
GLU	1.4	1.2	1.7	1.3	1.0	1.7	1.5	1.1
GLY	1	0	0	0	0	0	0	0
GLY	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	0	0	0	0	0	0	0	0
ILE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LEU	0	0	0	0	0	0	0	0
LEU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LYS	1	2	1	1	4	1	1	2
LYS	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
MET	0	0	0	0	0	0	0	0
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHE	0	0	0	0	0	0	0	0
PHE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PRO	0	0	0	0	0	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	0	0	0	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	0	0	0	0	0
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	0	0	0	0	0	0	0	0
VAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 31: Number of interactions and average atom contacts for interactions between charged atoms and polar side-chain atoms. Interactions are between pairs of α -helices.

[illegible]

Table 32: Number of interactions and average atom contacts for interactions between charged atoms and polar side-chain atoms. Interactions are between α -helices and β -sheets.

[illegible]

Table 33: Number of interactions and average atom contacts for interactions between charged atoms and polar side-chain atoms. Interactions are between β -sheets and α -helices.

[illegible]

Table 34: Number of interactions and average atom contacts for interactions between charged atoms and polar side-chain atoms. Interactions are between pairs of β -sheets.

[illegible]

APPENDIX E

Table 35: Total number of residue-residue interactions and average number of atom contacts for interactions between polar side-chain atoms.

	ARG	ASN	GLN	HIS	SER	THR	TRP	TYR
ARG	0	6	10	0	6	1	3	5
ARG	0.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0
ASN	6	56	37	10	40	31	3	28
ASN	1.0	1.1	1.0	1.2	1.0	1.2	1.0	1.1
GLN	10	37	20	7	26	22	6	12
GLN	1.0	1.0	1.1	1.0	1.1	1.0	1.0	1.1
HIS	0	10	7	32	22	11	1	17
HIS	0.0	1.2	1.0	1.0	1.0	1.0	1.0	1.1
SER	6	40	26	22	42	46	8	22
SER	1.0	1.0	1.1	1.0	1.0	1.0	1.0	1.0
THR	1	31	22	11	46	28	8	9
THR	1.0	1.2	1.0	1.0	1.0	1.0	1.0	1.0
TRP	3	3	6	1	8	8	0	4
TRP	1.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0
TYR	5	28	12	17	22	9	4	8
TYR	1.0	1.1	1.1	1.1	1.0	1.0	1.0	1.0

Table 36: Total number of residue-residue interactions and average number of atom contacts between secondary structures for interactions between polar side-chain atoms.

	ARG	ASN	GLN	HIS	SER	THR	TRP	TYR
ARG	0	3	3	0	2	0	1	2
ARG	0.0	1.0	1.0	0.0	1.0	0.0	1.0	1.0
ASN	3	2	10	2	12	8	1	8
ASN	1.0	1.0	1.0	1.0	1.1	1.2	1.0	1.0
GLN	3	10	8	3	8	9	1	6
GLN	1.0	1.0	1.0	1.0	1.0	1.1	1.0	1.2
HIS	0	2	3	16	8	5	0	4
HIS	0.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0
SER	2	12	8	8	10	13	6	3
SER	1.0	1.1	1.0	1.0	1.0	1.0	1.0	1.0
THR	0	8	9	5	13	12	3	3
THR	0.0	1.2	1.1	1.0	1.0	1.0	1.0	1.0
TRP	1	1	1	0	6	3	0	2
TRP	1.0	1.0	1.0	0.0	1.0	1.0	0.0	1.0
TYR	2	8	6	4	3	3	2	4
TYR	1.0	1.0	1.2	1.0	1.0	1.0	1.0	1.0

Table 37: Number of residue-residue interactions and average number of atom contacts between polar side-chain atoms. Interactions are between pairs of α -helices.

	ARG	ASN	GLN	HIS	SER	THR	TRP	TYR
ARG	0	2	1	0	1	0	0	0
ARG	0.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0
ASN	2	2	1	1	6	0	1	5
ASN	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0
GLN	1	1	4	2	2	1	1	0
GLN	1.0	1.0	1.0	1.0	1.0	2.0	1.0	0.0
HIS	0	1	2	6	7	0	0	3
HIS	0.0	1.0	1.0	1.0	1.0	0.0	0.0	1.0
SER	1	6	2	7	2	1	3	0
SER	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0
THR	0	0	1	0	1	0	3	3
THR	0.0	0.0	2.0	0.0	1.0	0.0	1.0	1.0
TRP	0	1	1	0	3	3	0	1
TRP	0.0	1.0	1.0	0.0	1.0	1.0	0.0	1.0
TYR	0	5	0	3	0	3	1	2
TYR	0.0	1.0	0.0	1.0	0.0	1.0	1.0	1.0

Table 38: Number of residue-residue interactions and average number of atom contacts between polar side-chain atoms. Interactions are between α -helices and β -sheets.

	ARG	ASN	GLN	HIS	SER	THR	TRP	TYR
ARG	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	1	0	3	0	2	1	0	0
ASN	1.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0
GLN	0	1	0	0	2	2	0	2
GLN	0.0	1.0	0.0	0.0	1.0	1.0	0.0	1.5
HIS	0	0	0	0	0	1	0	0
HIS	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
SER	0	2	0	0	1	0	1	1
SER	0.0	1.0	0.0	0.0	1.0	0.0	1.0	1.0
THR	0	2	0	0	1	0	0	0
THR	0.0	1.5	0.0	0.0	1.0	0.0	0.0	0.0
TRP	0	0	0	0	2	0	0	0
TRP	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
TYR	0	0	1	0	0	0	0	0
TYR	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0

Table 39: Number of residue-residue interactions and average number of atom contacts between polar side-chain atoms. Interactions are between β -sheets and α -helices.

	ARG	ASN	GLN	HIS	SER	THR	TRP	TYR
ARG	0	1	0	0	0	0	0	0
ARG	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	1	0	2	2	0	0
ASN	0.0	0.0	1.0	0.0	1.0	1.5	0.0	0.0
GLN	0	3	0	0	0	0	0	1
GLN	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0
HIS	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	2	2	0	1	1	2	0
SER	0.0	1.0	1.0	0.0	1.0	1.0	1.0	0.0
THR	0	1	2	1	0	0	0	0
THR	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	1	0	0	0
TRP	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
TYR	0	0	2	0	1	0	0	0
TYR	0.0	0.0	1.5	0.0	1.0	0.0	0.0	0.0

Table 40: Number of residue-residue interactions and average number of atom contacts between polar side-chain atoms. Interactions are between pairs of β -sheets.

	ARG	ASN	GLN	HIS	SER	THR	TRP	TYR
ARG	0	0	2	0	1	0	1	2
ARG	0.0	0.0	1.0	0.0	1.0	0.0	1.0	1.0
ASN	0	0	5	1	2	5	0	3
ASN	0.0	0.0	1.0	1.0	1.5	1.2	0.0	1.0
GLN	2	5	4	1	4	6	0	3
GLN	1.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0
HIS	0	1	1	10	1	4	0	1
HIS	0.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0
SER	1	2	4	1	6	11	0	2
SER	1.0	1.5	1.0	1.0	1.0	1.0	0.0	1.0
THR	0	5	6	4	11	12	0	0
THR	0.0	1.2	1.0	1.0	1.0	1.0	0.0	0.0
TRP	1	0	0	0	0	0	0	1
TRP	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
TYR	2	3	3	1	2	0	1	2
TYR	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0

APPENDIX F

Table 41: Total number of residue-residue interactions and average number of atom contacts between polar side-chain atoms and backbone oxygen atoms.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ARG	3	3	4	8	5	3	5	8	3	0	10	6	3	2	7	5	3	2	4	2
ARG	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
ASN	26	7	15	30	7	12	24	25	9	14	28	18	3	13	4	38	29	12	15	17
ASN	1.0	1.0	1.1	1.0	1.0	1.2	1.1	1.1	1.0	1.0	1.0	1.1	2.0	1.1	1.0	1.0	1.0	1.0	1.0	1.0
GLN	23	10	9	9	5	9	4	23	3	8	23	11	0	5	14	24	14	1	4	18
GLN	1.0	1.1	1.2	1.0	1.0	1.0	1.0	1.0	1.0	1.1	1.0	1.2	0.0	1.0	1.1	1.0	1.1	1.0	1.0	1.1
HIS	15	3	7	10	6	5	4	13	0	5	9	6	4	2	13	6	6	1	2	5
HIS	1.0	1.0	1.0	1.0	1.0	1.2	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
SER	42	10	13	31	6	13	21	30	8	6	29	18	1	17	10	42	21	2	10	24
SER	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
THR	28	13	14	21	6	6	15	30	7	13	14	18	2	11	14	25	22	10	12	20
THR	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
TRP	5	1	6	4	1	3	0	12	2	3	5	1	2	6	3	6	3	2	0	2
TRP	1.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0
TYR	5	0	7	8	1	4	2	9	2	4	1	11	1	2	14	10	3	0	2	12
TYR	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0

Table 42: Total number of residue-residue interactions and average number of atom contacts between secondary structures for polar side-chain atoms and backbone oxygen atoms.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ARG	1	1	0	0	1	0	1	2	1	0	3	1	2	1	1	1	2	1	1	1
ARG	1.0	1.0	0.0	0.0	1.0	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
ASN	2	2	0	1	2	2	3	2	1	4	8	1	2	1	0	6	1	0	5	6
ASN	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	2.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0
GLN	8	1	0	1	0	2	0	6	0	3	5	1	0	1	0	0	4	0	1	3
GLN	1.0	1.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	1.0	1.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	1.0
HIS	7	1	3	0	2	1	0	1	0	3	2	0	0	0	3	1	1	0	1	1
HIS	1.0	1.0	1.0	0.0	1.0	1.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	1.0	1.0
SER	4	0	1	1	0	1	1	6	5	0	4	2	0	3	1	4	5	0	1	4
SER	1.0	0.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0
THR	2	0	0	2	0	0	2	6	0	1	3	3	2	2	2	0	6	2	1	0
THR	1.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	0.0
TRP	3	0	1	0	1	0	0	1	0	3	4	0	0	1	1	1	1	0	0	1
TRP	1.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	1.0	1.0	1.0	1.0	0.0	0.0	1.0
TYR	2	0	0	2	0	1	1	3	0	2	1	1	0	1	1	1	1	0	1	2
TYR	1.0	0.0	0.0	1.0	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0

Table 43: Number of residue-residue interactions and average number of atom contacts between polar side-chain atoms and backbone oxygen atoms. Interactions are between pairs of α -helices.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ARG	1	1	0	0	0	0	1	0	1	0	3	0	0	1	0	1	1	1	1	0
ARG	1.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0
ASN	0	2	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	2
ASN	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0
GLN	3	0	0	0	0	1	0	0	0	1	4	0	0	0	0	0	0	0	0	2
GLN	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
HIS	2	0	2	0	1	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0
HIS	1.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	3	0	0	0	0	0	0	1	2	0	3	0	0	0	0	0	0	0	0	0
SER	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	1	0	0	0	0	0	0	1	0	0	2	0	0	0	0	0	0	0	0	0
THR	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	1
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
TYR	1	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	1	2
TYR	1.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0

Table 44: Number of residue-residue interactions and average number of atom contacts between polar side-chain atoms and backbone oxygen atoms. Interactions are between α -helices and β -sheets.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ARG	0	0	0	0	1	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	1	0	2	0	0	1	1	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	2.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
GLN	3	0	0	1	0	1	0	2	0	2	1	0	0	1	0	0	1	0	0	0
GLN	1.0	0.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0
HIS	1	1	1	0	0	0	0	1	0	3	0	0	0	0	3	0	1	0	0	1
HIS	1.0	1.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0
SER	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	1	0	0	2
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	1.0
THR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
TRP	0	0	0	0	1	0	0	1	0	0	0	0	0	1	1	1	1	0	0	0
TRP	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	1.0	0.0	0.0	0.0
TYR	0	0	0	1	0	0	0	2	0	1	1	0	0	0	0	0	1	0	0	0
TYR	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0

Table 45: Number of residue-residue interactions and average number of atom contacts between polar side-chain atoms and backbone oxygen atoms. Interactions are between α -helices and β -sheets.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ARG	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	1	0	0	0	0	1	0	1	0	2	2	1	0	0	0	2	0	0	1	0
ASN	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
SER	1	0	0	0	0	0	0	0	3	0	1	0	0	1	0	1	0	0	0	0
SER	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0
THR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
TRP	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
TRP	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	1	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0
TYR	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0

Table 46: Number of residue-residue interactions and average number of atom contacts between polar side-chain atoms and backbone oxygen atoms. Interactions are between pairs of β -sheets.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ARG	0	0	0	0	0	0	0	2	0	0	0	0	1	0	0	0	1	0	0	1
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0
ASN	1	0	0	1	2	1	3	1	1	1	5	0	0	1	0	3	0	0	3	4
ASN	1.0	0.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	1.0
GLN	2	1	0	0	0	0	0	4	0	0	0	0	0	0	0	0	3	0	1	1
GLN	1.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0
HIS	4	0	0	0	1	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
HIS	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
SER	0	0	1	1	0	1	1	3	0	0	0	2	0	2	1	2	4	0	1	2
SER	0.0	0.0	1.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0
THR	1	0	0	2	0	0	2	5	0	1	1	3	2	2	2	0	2	2	1	0
THR	1.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	0.0
TRP	2	0	1	0	0	0	0	0	0	1	3	0	0	0	0	0	0	0	0	0
TRP	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0

Table 47: Total number of residue-residue interactions and average number of atom contacts for polar side-chain atoms and backbone nitrogen atoms.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ARG	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	21	4	23	18	7	10	19	39	6	5	13	26	2	8	3	25	16	9	17	20
ASN	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
GLN	4	4	11	9	2	1	2	9	3	2	3	5	0	1	1	13	5	0	4	5
GLN	1.0	1.0	1.1	1.1	1.0	1.0	1.0	1.2	1.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0
HIS	1	0	1	5	1	0	1	2	0	0	2	3	0	1	0	7	4	0	0	2
HIS	1.0	0.0	1.0	1.0	1.0	0.0	1.0	1.0	0.0	0.0	1.0	1.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	1.0
SER	21	5	10	26	2	12	23	19	0	4	11	9	3	14	1	37	20	4	15	17
SER	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
THR	21	4	13	20	5	7	16	14	3	1	6	3	3	4	1	16	10	3	6	12
THR	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
TRP	0	0	1	0	0	0	1	5	1	1	6	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	1.0	0.0	0.0	0.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	4	5	4	13	5	2	2	12	2	2	2	3	0	0	6	9	5	0	1	2
TYR	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0	1.0	1.0

Table 48: Total number of residue-residue interactions and average number of atom contacts between secondary structures for polar side-chain atoms and backbone nitrogen atoms.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	1	1	2	1	2	4	0	0	4	1	0	0	2	2	2	1	1	1
ASN	0.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
GLN	1	1	0	2	1	0	0	1	0	0	1	0	0	1	1	1	0	0	1	2
GLN	1.0	1.0	0.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	1.0	1.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	1
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0
SER	2	2	1	0	0	0	1	4	0	1	2	0	0	5	0	8	4	0	2	1
SER	1.0	1.0	1.0	0.0	0.0	0.0	1.0	1.0	0.0	1.0	1.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0
THR	2	0	0	1	1	0	1	7	0	0	2	0	0	0	1	2	2	0	0	1
THR	1.0	0.0	0.0	1.0	1.0	0.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	1.0
TRP	0	0	1	0	0	0	0	2	0	1	1	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	1	0	3	0	0	0	2	0	1	1	2	0	0	1	0	1	0	0	0
TYR	0.0	1.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0

Table 49: Number of residue-residue interactions and average number of atom contacts between polar side-chain atoms and backbone nitrogen atoms. Interactions are between pairs of α -helices.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0
ASN	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
SER	2	1	0	0	0	0	0	1	0	0	1	0	0	1	0	1	0	0	0	0
SER	1.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0
THR	1	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0
THR	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	1	0	2	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
TYR	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 50: Number of residue-residue interactions and average number of atom contacts between polar side-chain atoms and backbone nitrogen atoms. Interactions are between α -helices and β -sheets.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	2	0	0	1	0	0	1	0	0	0	0	0	1	0	1	0
ASN	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0
GLN	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
GLN	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	0	1	0	0	1	0	0	1	0	1	0	0	1	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0
THR	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
THR	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	1	0	0	0
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0

Table 51: Number of residue-residue interactions and average number of atom contacts between polar side-chain atoms and backbone nitrogen atoms. Interactions are between β -sheets and α -helices.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	1	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0
GLN	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLN	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
SER	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	2	3	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
THR	0	0	0	0	1	0	0	4	0	0	0	0	0	0	0	1	0	0	0	0
THR	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
TYR	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 52: Number of residue-residue interactions and average number of atom contacts between polar side-chain atoms and backbone nitrogen atoms. Interactions are between pairs of β -sheets.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	1	0	0	1	2	3	0	0	3	0	0	0	0	1	0	1	0	1
ASN	0.0	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	1.0
GLN	1	0	0	1	0	0	0	1	0	0	1	0	0	1	1	0	0	0	1	0
GLN	1.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	1.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	1	1	0	0	0	0	1	0	1	0	0	0	3	0	4	1	0	1	1
SER	0.0	1.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0
THR	0	0	0	1	0	0	1	2	0	0	1	0	0	0	0	0	2	0	0	1
THR	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0
TRP	0	0	1	0	0	0	0	2	0	1	1	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	0	0	0	0	0	0	1	0	1	0	0	1	0	0	0	0	0
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0

APPENDIX G

Table 53: Total number of residue-residue interactions and average atom contacts for interactions between backbone atoms.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	115	29	41	74	19	35	63	82	14	55	104	77	17	50	29	75	43	18	28	71
ALA	1.2	1.3	1.3	1.3	1.3	1.2	1.3	1.2	1.1	1.4	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.2	1.2	1.3
ARG	28	17	15	28	9	12	13	29	2	22	32	29	7	24	8	22	27	5	19	17
ARG	1.3	1.5	1.3	1.3	1.2	1.3	1.2	1.5	1.5	1.3	1.2	1.2	1.3	1.3	1.2	1.3	1.2	1.4	1.2	1.1
ASN	43	11	40	27	11	11	27	40	10	21	54	40	6	25	9	21	32	11	25	21
ASN	1.2	1.3	1.2	1.1	1.2	1.2	1.1	1.4	1.1	1.5	1.4	1.2	1.2	1.2	1.3	1.4	1.3	1.3	1.2	1.2
ASP	53	18	23	50	12	24	25	37	11	26	42	52	12	28	10	50	40	9	14	26
ASP	1.2	1.2	1.5	1.2	1.2	1.2	1.2	1.3	1.4	1.3	1.3	1.1	1.1	1.1	1.3	1.3	1.2	1.3	1.4	1.6
CYS	22	9	9	9	5	9	17	21	3	6	22	10	2	7	7	13	10	2	6	13
CYS	1.3	1.3	1.7	1.6	1.0	1.1	1.5	1.3	1.3	1.7	1.5	1.4	2.0	1.1	1.4	1.2	1.0	1.0	1.5	1.1
GLN	32	21	13	23	7	19	30	26	5	13	47	28	14	19	15	26	17	15	13	29
GLN	1.2	1.3	1.3	1.4	1.4	1.2	1.3	1.1	1.0	1.4	1.3	1.2	1.3	1.4	1.5	1.2	1.5	1.1	1.7	1.2
GLU	55	17	25	28	12	34	27	32	8	26	55	45	7	22	9	28	28	10	21	30
GLU	1.4	1.3	1.2	1.3	1.1	1.2	1.3	1.2	1.2	1.3	1.2	1.3	1.5	1.3	1.4	1.2	1.2	1.5	1.3	
GLY	98	37	42	51	20	27	30	99	17	22	76	61	20	29	24	53	45	15	36	58
GLY	1.3	1.5	1.4	1.4	1.4	1.6	1.3	1.4	1.3	1.4	1.4	1.6	1.6	1.4	1.3	1.4	1.3	1.7	1.5	1.4
HIS	12	3	10	13	7	5	9	16	9	3	15	8	4	12	8	6	8	3	5	8
HIS	1.4	1.3	1.2	1.3	1.3	1.2	1.0	1.4	1.2	1.7	1.1	1.4	1.2	1.4	1.7	1.3	1.5	1.0	1.2	1.0
ILE	62	18	24	25	7	13	22	27	4	28	41	32	9	28	9	27	29	5	14	20
ILE	1.3	1.1	1.3	1.2	1.1	1.2	1.3	1.3	1.2	1.2	1.3	1.2	1.1	1.3	1.3	1.1	1.2	1.0	1.3	1.3
LEU	94	33	57	43	24	46	68	71	16	42	79	61	19	45	25	62	50	16	21	65
LEU	1.2	1.2	1.3	1.2	1.2	1.2	1.3	1.3	1.4	1.4	1.3	1.2	1.3	1.3	1.6	1.2	1.3	1.2	1.4	1.2
LYS	83	22	43	61	11	25	57	52	8	37	61	51	14	46	12	33	22	14	20	47
LYS	1.2	1.2	1.5	1.4	1.4	1.4	1.2	1.2	1.2	1.2	1.4	1.3	1.4	1.3	1.2	1.4	1.7	1.2	1.1	1.3
MET	19	6	10	13	1	11	14	15	5	6	20	18	6	14	3	13	13	1	17	11
MET	1.2	1.3	1.1	1.2	1.0	1.4	1.2	1.4	1.6	1.5	1.2	1.2	1.5	1.3	1.0	1.5	1.5	2.0	1.2	1.2
PHE	48	22	21	28	6	17	32	31	15	28	38	47	15	16	17	22	25	9	12	32
PHE	1.2	1.3	1.2	1.2	1.5	1.2	1.2	1.2	1.5	1.2	1.4	1.3	1.1	1.5	1.3	1.3	1.3	1.1	1.3	1.3
PRO	19	8	6	5	4	10	6	22	7	8	24	13	2	15	3	16	14	2	14	14
PRO	1.1	1.2	1.2	1.0	1.2	1.0	1.0	1.3	1.1	1.2	1.2	1.3	1.0	1.1	1.3	1.2	1.2	1.5	1.2	1.3
SER	73	25	23	55	12	25	31	44	9	29	55	29	18	23	19	48	38	9	25	61
SER	1.2	1.1	1.2	1.3	1.3	1.3	1.2	1.4	1.3	1.3	1.4	1.6	1.3	1.1	1.3	1.2	1.3	1.3	1.4	1.3
THR	45	27	24	36	9	15	22	38	11	24	44	25	9	23	13	43	26	14	20	30
THR	1.2	1.1	1.1	1.3	1.1	1.2	1.4	1.2	1.3	1.4	1.2	1.3	1.2	1.3	1.2	1.2	1.1	1.1	1.1	1.3
TRP	21	5	6	8	2	8	9	16	2	2	17	14	3	7	3	10	6	5	9	21
TRP	1.1	1.0	1.2	1.2	1.0	1.5	1.1	1.3	1.5	1.0	1.4	1.4	1.0	1.0	1.3	1.4	1.3	1.4	1.3	1.3
TYR	22	17	28	19	6	12	24	37	5	15	22	19	13	12	10	27	21	11	16	22
TYR	1.3	1.5	1.2	1.4	1.5	1.2	1.3	1.2	1.0	1.3	1.4	1.3	1.2	1.2	1.4	1.2	1.2	1.4	1.2	1.2
VAL	67	15	27	30	16	35	26	56	10	20	61	47	11	34	21	66	30	22	18	56
VAL	1.3	1.2	1.3	1.3	1.4	1.2	1.2	1.2	1.1	1.1	1.2	1.3	1.3	1.3	1.3	1.2	1.2	1.3	1.2	1.2

Table 54: Total number of residue-residue interactions and average atom contacts for interactions between secondary structures involving backbone atoms.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	27	12	6	7	2	9	4	36	6	38	28	13	11	17	11	29	17	7	17	49
ALA	1.0	1.3	1.2	1.6	1.0	1.0	1.2	1.1	1.0	1.2	1.2	1.1	1.2	1.1	1.3	1.0	1.2	1.0	1.2	1.2
ARG	10	0	3	6	0	3	4	5	3	9	2	4	6	4	3	8	13	3	6	11
ARG	1.2	0.0	1.3	1.7	0.0	1.0	1.0	2.0	1.0	1.3	1.0	1.2	1.3	1.0	1.0	1.1	1.1	1.0	1.2	1.2
ASN	9	5	4	2	2	3	8	15	1	7	15	3	5	7	1	3	5	1	7	7
ASN	1.1	1.0	1.2	2.0	1.5	1.3	1.2	1.4	1.0	1.0	1.3	1.0	1.0	1.1	2.0	1.3	1.0	1.0	1.4	1.9
ASP	6	4	4	1	0	6	3	13	2	6	19	8	1	4	0	5	13	1	4	8
ASP	1.0	1.5	1.2	1.0	0.0	1.0	1.3	1.5	1.0	1.3	1.1	1.2	1.0	1.0	0.0	1.0	1.2	2.0	2.0	1.4
CYS	6	1	3	0	0	5	3	11	2	4	10	4	2	10	1	2	4	0	1	10
CYS	1.2	1.0	1.0	0.0	0.0	1.2	1.0	1.2	1.5	1.8	1.4	1.5	1.0	1.1	1.0	1.5	1.0	0.0	2.0	1.3
GLN	12	4	1	9	1	3	2	7	0	6	14	5	0	8	2	7	11	2	4	10
GLN	1.0	1.2	1.0	1.0	1.0	1.3	1.0	1.0	0.0	1.2	1.1	1.2	0.0	1.2	1.0	1.1	1.2	1.5	1.2	1.0
GLU	8	3	7	1	0	4	4	5	3	10	8	10	3	3	2	7	7	3	7	12
GLU	1.1	1.0	1.1	1.0	0.0	1.2	1.5	1.6	1.0	1.3	1.2	1.2	1.3	1.0	1.0	1.3	1.0	1.7	1.3	1.2
GLY	43	4	19	25	5	7	7	44	4	27	39	11	7	14	9	24	21	6	15	46
GLY	1.3	1.0	1.4	1.4	1.6	1.1	1.1	1.4	1.0	1.2	1.4	1.4	1.3	1.1	1.2	1.5	1.2	1.2	1.3	1.2
HIS	8	4	1	3	2	1	4	6	4	4	5	3	0	2	0	4	5	0	2	6
HIS	1.0	1.8	1.0	1.0	1.0	1.0	1.0	1.7	1.0	1.2	1.2	1.0	0.0	1.0	0.0	1.0	1.6	0.0	1.0	1.0
ILE	37	6	8	1	4	9	9	24	5	37	34	16	5	13	3	9	28	14	22	53
ILE	1.2	1.0	1.1	1.0	1.5	1.0	1.1	1.2	1.2	1.1	1.1	1.2	1.0	1.1	1.0	1.1	1.1	1.1	1.1	1.2
LEU	20	6	12	13	11	14	9	32	7	38	41	17	5	15	5	17	15	9	11	52
LEU	1.1	1.0	1.0	1.2	1.2	1.1	1.0	1.1	1.1	1.2	1.1	1.2	1.0	1.1	1.0	1.1	1.0	1.0	1.4	1.2
LYS	17	3	6	12	3	6	10	10	1	10	13	19	6	4	1	12	9	0	8	16
LYS	1.2	1.0	1.2	1.2	1.0	1.0	1.1	1.1	1.0	1.1	1.2	1.3	1.2	2.2	1.0	1.0	1.0	0.0	1.4	1.1
MET	7	2	2	2	0	1	2	7	2	5	9	6	1	2	1	4	10	0	7	12
MET	1.3	1.5	1.0	1.0	0.0	1.0	1.0	1.4	1.0	1.0	1.0	1.3	2.0	1.5	1.0	1.2	1.0	0.0	1.1	1.4
PHE	5	9	3	6	7	6	8	18	5	26	24	9	3	14	1	9	10	0	7	25
PHE	1.2	1.2	1.3	1.5	1.0	1.3	1.4	1.2	1.4	1.1	1.2	1.2	2.3	1.1	1.0	1.0	1.1	0.0	1.1	1.2
PRO	0	1	1	1	0	1	1	9	0	2	9	3	0	3	0	3	4	0	6	5
PRO	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.6	0.0	1.0	1.0	1.0	0.0	1.7	0.0	1.3	1.2	0.0	1.5	1.0
SER	21	8	2	3	7	6	10	29	3	18	17	14	8	11	5	21	14	10	16	24
SER	1.1	1.0	1.0	1.0	1.4	1.2	1.4	1.2	1.3	1.2	1.3	1.4	1.4	1.1	1.0	1.0	1.1	1.3	1.7	1.1
THR	14	17	2	6	3	7	11	18	4	24	19	10	9	15	3	24	21	4	14	27
THR	1.2	1.3	1.5	1.0	1.0	1.1	1.1	1.3	1.2	1.2	1.1	1.1	1.2	1.3	1.0	1.1	1.0	1.2	1.2	1.2
TRP	5	4	0	2	0	4	3	8	1	5	11	0	1	0	1	5	5	1	8	12
TRP	1.0	1.5	0.0	1.5	0.0	1.2	1.0	1.1	1.0	1.0	1.2	0.0	1.0	0.0	1.0	1.4	1.4	1.0	1.4	1.5
TYR	18	5	6	5	1	7	6	16	2	26	16	9	1	11	0	16	12	10	10	25
TYR	1.2	1.0	1.3	1.2	1.0	1.4	1.3	1.4	1.0	1.3	1.1	1.2	1.0	1.1	0.0	1.3	1.2	1.3	1.0	1.1
VAL	46	14	10	12	13	24	9	40	7	42	50	19	8	23	3	25	25	11	21	87
VAL	1.1	1.2	1.2	1.0	1.2	1.0	1.0	1.1	1.1	1.2	1.1	1.1	1.1	1.1	1.0	1.0	1.1	1.3	1.0	1.1

Table 55: Number of residue-residue interactions and average atom contacts for interactions between backbone atoms. Interactions are between pairs of α -helices.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	1	0	0	0	0	0	0	4	0	2	3	2	0	0	0	2	0	0	1	3
ALA	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.5	1.3	1.0	0.0	0.0	0.0	1.0	0.0	0.0	3.0	1.3
ARG	0	0	0	2	0	0	0	0	0	1	0	0	0	0	0	3	1	0	0	0
ARG	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
ASN	2	0	0	0	0	0	1	2	0	0	2	2	2	0	0	0	0	0	1	2
ASN	1.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	0.0	0.0	2.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0
ASP	1	2	0	0	0	1	1	1	0	0	4	1	0	0	0	0	0	0	1	1
ASP	1.0	1.5	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.0
CYS	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	1	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	1.0	0.0	2.0	0.0	0.0	0.0	0.0
GLN	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	1
GLN	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0	0.0	1.0
GLU	0	0	1	0	0	0	0	1	0	0	0	1	0	0	0	1	0	0	1	1
GLU	0.0	0.0	1.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	2.0	0.0	0.0	1.0	1.0
GLY	3	1	2	1	0	0	2	14	3	2	2	2	0	1	2	2	1	0	0	1
GLY	1.0	1.0	2.0	2.0	0.0	0.0	1.0	1.7	1.0	1.0	2.0	1.5	0.0	1.0	1.0	2.0	1.0	0.0	0.0	1.0
HIS	3	0	0	1	0	0	0	3	0	0	0	0	0	0	0	2	0	0	0	2
HIS	1.0	0.0	0.0	1.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0
ILE	1	1	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	1	4	3
ILE	1.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.2	1.3
LEU	2	1	2	2	2	0	0	3	0	0	2	1	0	2	0	1	0	0	0	3
LEU	1.5	1.0	1.0	1.5	1.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	1.3
LYS	1	0	2	0	0	0	1	2	0	1	2	0	0	1	0	0	0	0	1	3
LYS	1.0	0.0	1.5	0.0	0.0	0.0	1.0	1.0	0.0	1.0	1.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	1.0	1.0
MET	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
MET	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHE	0	0	0	1	0	0	0	1	0	0	2	1	2	1	0	1	0	0	0	0
PHE	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	3.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0
PRO	0	0	0	0	0	1	0	2	0	1	3	0	0	1	0	1	0	0	2	0
PRO	0.0	0.0	0.0	0.0	0.0	1.0	0.0	2.0	0.0	1.0	1.0	0.0	0.0	2.0	0.0	1.0	0.0	0.0	2.0	0.0
SER	1	0	0	0	1	0	1	1	0	0	5	0	0	2	0	0	0	1	4	0
SER	1.0	0.0	0.0	0.0	1.0	0.0	1.0	4.0	0.0	0.0	1.2	0.0	0.0	1.0	0.0	0.0	0.0	1.0	2.2	0.0
THR	1	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
THR	1.0	2.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	0	1	0	1	0	1	1	0	0	0	0	1	0	0	3	4
TRP	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0	2.0
TYR	1	0	1	1	0	0	1	0	0	1	2	1	0	0	0	4	0	3	0	2
TYR	1.0	0.0	1.0	1.0	0.0	0.0	2.0	0.0	0.0	1.0	1.5	1.0	0.0	0.0	0.0	1.8	0.0	1.3	0.0	1.0
VAL	3	0	2	1	0	0	0	2	0	2	2	0	0	1	0	0	0	4	2	7
VAL	1.0	0.0	1.0	1.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	1.0	1.4

Table 56: Number of residue-residue interactions and average atom contacts for interactions between backbone atoms. Interactions are between α -helices and β -sheets.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	1	0	1	0	0	0	4	0	0	1	1	1	1	4	1	0	0	0	2
ALA	0.0	3.0	0.0	4.0	0.0	0.0	0.0	1.2	0.0	0.0	1.0	1.0	2.0	1.0	1.2	1.0	0.0	0.0	0.0	1.5
ARG	2	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	2	0
ARG	1.5	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
ASN	1	2	0	1	0	0	0	1	0	0	1	0	0	0	1	0	1	0	2	1
ASN	2.0	1.0	0.0	2.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	2.0	0.0	1.0	0.0	2.0	4.0
ASP	0	0	1	0	0	0	1	4	0	1	1	0	0	0	0	0	2	0	0	1
ASP	0.0	0.0	2.0	0.0	0.0	0.0	2.0	2.0	0.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0
CYS	0	0	0	0	0	0	0	2	0	1	0	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	1	0	1	0	0	1	0	0	0	0	0	0	0	0	0	2	0	0	0	0
GLN	1.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0
GLU	0	0	1	0	0	0	1	1	0	0	0	0	0	1	0	0	0	0	0	0
GLU	0.0	0.0	1.0	0.0	0.0	0.0	3.0	2.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	1	2	0	0	0	6	0	4	3	0	0	0	0	1	3	0	0	2
GLY	0.0	0.0	1.0	1.0	0.0	0.0	0.0	1.2	0.0	1.2	1.7	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	1.5
HIS	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	3	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0
ILE	1	0	0	0	0	1	0	1	0	0	0	1	0	0	1	0	2	0	0	1
ILE	1.0	0.0	0.0	0.0	0.0	1.0	0.0	2.0	0.0	0.0	0.0	2.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0
LEU	1	1	0	1	0	2	1	3	0	1	2	1	1	0	1	1	0	0	0	2
LEU	2.0	1.0	0.0	2.0	0.0	1.5	1.0	1.0	0.0	1.0	1.0	2.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	2.5
LYS	1	0	0	1	0	1	1	1	0	0	2	2	0	0	0	0	1	0	0	0
LYS	1.0	0.0	0.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	1.0	1.5	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
MET	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHE	0	0	0	1	1	0	0	2	0	0	1	0	0	0	0	1	1	0	0	0
PHE	0.0	0.0	0.0	2.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
PRO	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	1	3	0	0	0	0	1	0	0	1	1	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
THR	1	1	1	1	0	0	2	3	0	0	0	0	0	0	0	0	1	0	0	0
THR	2.0	2.0	2.0	1.0	0.0	0.0	1.0	1.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
TRP	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	5
VAL	2.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	1.0

ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
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	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	2	1	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	2
ALA	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0
ARG	1	0	1	0	0	0	1	1	0	0	0	0	0	0	0	0	1	0	0	0
ARG	1.0	0.0	1.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
ASN	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	1	0	0	1
ASN	0.0	0.0	0.0	0.0	0.0	2.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0
ASP	1	0	1	0	0	0	0	0	0	0	1	0	0	1	0	0	1	0	0	0
ASP	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0
CYS	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	1	0	1	0	1	2	1	0	1	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	2.0	0.0	1.0	0.0	2.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0
GLU	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
GLY	5	1	1	5	0	0	1	4	0	3	1	1	0	0	1	1	3	0	0	1
GLY	1.2	1.0	1.0	1.2	0.0	0.0	1.0	1.2	0.0	1.0	1.0	3.0	0.0	0.0	1.0	1.0	1.3	0.0	0.0	1.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
ILE	0	0	0	1	1	0	0	4	0	0	1	0	0	0	0	0	2	0	0	1
ILE	0.0	0.0	0.0	1.0	1.0	0.0	0.0	1.2	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0
LEU	0	0	0	1	0	0	0	0	1	0	5	1	0	0	0	0	0	0	0	0
LEU	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LYS	1	0	0	0	0	0	0	0	0	1	2	1	0	0	0	0	1	0	0	0
LYS	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	2.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
MET	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
MET	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
PHE	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0
PHE	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PRO	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
PRO	0.0	0.0	1.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	1	0	0	0	0	1	0	1	0	0	1	2	0	1	0	0	0	0	0	0
SER	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	2.0	1.5	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	0	0	0	1
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	1	2	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0
TYR	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	1	0	1	1	0	1	0	1	1	0	1	0	0	0	0	0	0	0	0	1
VAL	1.0	0.0	2.0	1.0	0.0	1.0	0.0	2.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0

Table 58: Number of residue-residue interactions and average atom contacts for interactions between backbone atoms. Interactions are between pairs of β -sheets.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	26	9	5	6	2	9	4	28	6	36	23	10	10	16	7	26	16	7	16	42
ALA	1.0	1.2	1.2	4.2	1.0	1.0	1.2	1.1	1.0	1.2	1.3	1.1	1.1	1.1	1.3	1.0	1.2	1.0	1.1	1.2
ARG	7	0	2	4	0	3	3	3	3	8	1	4	6	4	3	5	11	3	4	11
ARG	1.1	0.0	1.5	1.8	0.0	1.0	1.0	2.3	1.0	1.2	1.0	1.2	1.3	1.0	1.0	1.2	1.1	1.0	1.2	1.2
ASN	6	3	4	1	2	2	7	11	1	7	12	1	3	7	0	3	3	1	4	3
ASN	1.0	1.0	1.2	2.0	1.5	1.0	1.1	1.5	1.0	1.0	1.2	1.0	1.1	1.0	0.0	1.3	1.0	1.0	1.0	1.3
ASP	4	2	2	1	0	5	1	8	2	5	13	7	1	3	0	5	10	1	3	6
ASP	1.0	1.5	1.0	1.0	0.0	1.0	1.0	1.4	1.0	1.2	1.2	1.3	1.0	1.0	0.0	1.0	1.2	2.0	2.3	1.2
CYS	6	1	3	0	0	5	3	9	2	3	9	4	2	8	1	1	4	0	1	10
CYS	1.2	1.0	1.0	0.0	0.0	1.2	1.0	1.2	1.5	2.0	1.3	1.5	1.0	1.1	1.0	1.0	1.0	0.0	2.0	1.3
GLN	11	4	0	8	1	1	2	6	0	5	12	4	0	7	1	5	11	1	4	9
GLN	1.0	1.2	0.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.2	1.2	0.0	1.3	1.0	1.0	1.2	1.0	1.2	1.0
GLU	8	3	5	0	0	4	2	3	3	10	8	9	3	2	2	5	7	3	6	11
GLU	1.1	1.0	1.2	0.0	0.0	1.2	1.0	1.3	1.0	1.3	1.2	1.2	1.3	1.0	1.0	1.2	1.0	1.7	1.3	1.2
GLY	35	2	15	17	5	7	4	20	1	18	33	8	7	13	6	20	14	6	15	42
GLY	1.3	1.0	1.3	1.4	1.6	1.1	1.2	1.2	1.0	1.3	1.3	1.1	1.3	1.1	1.3	1.5	1.2	1.2	1.3	1.2
HIS	3	4	1	2	2	1	4	3	4	4	4	3	0	2	0	2	2	0	2	3
HIS	1.0	1.8	1.0	1.0	1.0	1.0	1.0	1.3	1.0	1.2	1.2	1.0	0.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0
ILE	35	5	8	0	3	8	9	18	5	37	33	15	5	13	1	9	24	13	18	48
ILE	1.2	1.0	1.1	0.0	1.7	1.0	1.1	1.1	1.2	1.1	1.1	1.1	1.0	1.1	1.0	1.1	1.1	1.1	1.1	1.2
LEU	17	4	10	9	9	12	8	26	6	37	32	14	4	13	4	15	15	9	11	47
LEU	1.0	1.0	1.0	1.1	1.2	1.1	1.0	1.1	1.2	1.2	1.1	1.1	1.0	1.2	1.0	1.1	1.0	1.0	1.4	1.1
LYS	14	3	4	11	3	5	8	7	1	8	7	16	6	3	1	12	7	0	7	13
LYS	1.1	1.0	1.0	1.3	1.0	1.0	1.1	1.1	1.0	1.1	1.4	1.2	1.2	2.3	1.0	1.0	1.0	0.0	1.4	1.1
MET	6	2	0	2	0	1	2	7	2	5	8	6	1	2	1	3	10	0	7	12
MET	1.3	1.5	0.0	1.0	0.0	1.0	1.0	1.4	1.0	1.0	1.0	1.3	2.0	1.5	1.0	1.3	1.0	0.0	1.1	1.4
PHE	5	9	3	4	6	6	7	15	4	26	21	8	1	13	1	7	9	0	7	25
PHE	1.2	1.2	1.3	1.5	1.0	1.3	1.4	1.3	1.2	1.1	1.2	1.2	1.0	1.1	1.0	1.0	1.1	0.0	1.1	1.2
PRO	0	1	0	1	0	0	1	5	0	1	6	3	0	2	0	2	4	0	4	5
PRO	0.0	1.0	0.0	1.0	0.0	0.0	1.0	1.4	0.0	1.0	1.0	1.0	0.0	1.5	0.0	1.5	1.2	0.0	1.2	1.0
SER	19	8	2	3	6	5	8	24	3	18	11	12	7	8	5	20	13	9	12	24
SER	1.1	1.0	1.0	1.0	1.5	1.2	1.4	1.2	1.3	1.2	1.3	1.4	1.4	1.1	1.0	1.0	1.1	1.3	1.5	1.1
THR	12	15	1	5	3	7	9	12	4	24	19	10	9	15	3	23	20	4	14	26
THR	1.2	1.2	1.0	1.0	1.0	1.1	1.1	1.2	1.2	1.2	1.1	1.1	1.2	1.3	1.0	1.1	1.0	1.2	1.2	1.2
TRP	4	4	0	2	0	3	3	7	1	4	10	0	1	0	1	4	5	1	5	8
TRP	1.0	1.5	0.0	1.5	0.0	1.3	1.0	1.1	1.0	1.0	1.2	0.0	1.0	0.0	1.0	1.5	1.4	1.0	1.0	1.2
TYR	17	4	3	4	1	7	5	15	2	24	14	8	1	9	0	12	12	7	10	23
TYR	1.2	1.0	1.7	1.2	1.0	1.4	1.2	1.4	1.0	1.3	1.1	1.2	1.0	1.1	0.0	1.2	1.2	1.3	1.0	1.1
VAL	40	14	6	10	13	23	9	37	6	40	47	19	8	22	3	25	24	7	19	74
VAL	1.1	1.2	1.0	1.0	1.2	1.0	1.0	1.1	1.2	1.2	1.1	1.1	1.1	1.1	1.0	1.0	1.0	1.4	1.1	1.1

Table 59: Total number of residue-residue interactions and average atom contacts for interactions between backbone atoms and hydrophobic side-chain atoms.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	103	29	17	35	27	35	44	0	16	93	104	58	36	51	49	67	56	22	49	98
ALA	1.2	1.4	1.4	1.5	1.3	1.5	1.3	0.0	1.2	1.7	1.7	1.7	2.2	1.9	1.7	1.3	1.5	1.7	1.7	1.5
ARG	26	11	5	7	5	15	21	0	6	21	50	10	3	23	17	12	16	19	13	19
ARG	1.2	1.7	1.6	1.6	2.0	1.5	1.6	0.0	2.2	2.0	1.5	1.7	2.0	1.9	1.8	1.1	1.4	1.5	3.0	1.6
ASN	32	15	27	22	16	23	29	0	13	29	41	46	16	28	18	28	17	14	43	41
ASN	1.1	1.7	1.4	1.5	1.6	1.5	1.5	0.0	1.1	1.5	1.6	1.8	1.9	1.9	1.7	1.4	1.3	2.0	2.4	1.5
ASP	51	35	23	7	14	16	17	0	14	30	50	71	9	28	21	34	39	17	48	34
ASP	1.2	1.8	1.2	1.1	1.6	1.3	1.7	0.0	1.1	1.6	1.9	1.6	1.7	1.8	1.9	1.1	1.4	1.9	1.5	2.3
CYS	7	6	5	13	99	7	3	0	13	8	33	12	7	13	8	11	8	8	20	23
CYS	1.1	1.0	1.2	2.5	1.7	1.3	1.7	0.0	1.7	1.4	1.5	1.8	1.6	1.5	1.5	1.3	1.2	1.6	1.6	1.3
GLN	38	16	9	24	12	16	20	0	7	15	28	27	12	21	15	14	13	17	9	33
GLN	1.2	2.1	1.1	1.3	1.7	1.4	1.8	0.0	1.0	1.6	1.6	1.4	1.5	2.0	1.8	1.1	1.2	2.0	2.1	1.8
GLU	45	23	20	20	13	10	23	0	7	34	46	52	16	30	33	32	18	8	29	27
GLU	1.2	1.6	1.4	1.5	1.8	1.4	1.3	0.0	1.4	1.9	1.5	1.6	1.6	1.6	2.0	1.2	1.8	1.9	1.7	1.6
GLY	73	25	37	50	28	31	40	0	25	72	130	55	26	70	60	47	72	45	84	121
GLY	1.6	2.2	1.7	1.4	1.5	1.5	1.6	0.0	1.4	2.2	1.8	2.1	2.2	2.4	1.9	1.4	1.8	2.4	3.3	2.0
HIS	12	4	10	6	4	3	7	0	8	12	25	6	6	22	9	10	13	7	11	13
HIS	1.2	1.5	1.1	1.2	1.8	2.0	1.6	0.0	1.1	1.3	1.4	2.5	2.0	2.2	1.6	1.1	1.4	3.0	1.3	1.5
ILE	42	16	11	19	8	19	16	0	14	29	58	27	18	37	13	24	20	16	28	37
ILE	1.3	1.4	1.0	1.2	1.2	1.8	1.5	0.0	1.8	1.5	1.3	1.3	1.4	1.4	1.7	1.2	1.5	1.8	2.0	1.5
LEU	69	30	9	17	14	29	16	0	14	70	106	48	26	59	30	42	34	29	43	84
LEU	1.3	1.4	1.6	1.1	1.6	1.3	1.6	0.0	1.7	1.7	1.6	1.9	1.5	1.6	1.9	1.4	1.4	1.7	1.3	1.4
LYS	39	23	25	39	10	24	30	0	8	38	51	44	23	25	36	25	26	22	36	45
LYS	1.3	1.6	1.5	1.5	2.2	1.3	1.7	0.0	1.4	1.9	1.6	1.8	2.0	2.0	1.8	1.4	1.5	1.8	1.8	1.5
MET	15	14	4	4	4	9	2	0	8	12	25	8	5	13	6	10	4	8	9	15
MET	1.1	1.6	1.0	1.0	1.5	1.8	1.5	0.0	1.1	1.6	1.4	1.6	1.6	2.2	2.2	1.0	1.2	1.4	1.6	1.3
PHE	31	11	16	9	16	7	9	0	7	30	45	28	15	26	14	23	13	18	18	42
PHE	1.3	2.1	1.1	1.1	1.8	1.9	1.1	0.0	1.4	1.7	1.4	1.3	1.4	1.6	1.6	1.2	1.5	1.3	1.7	1.5
PRO	32	20	8	9	8	28	13	0	8	24	55	20	6	30	21	18	25	13	29	45
PRO	1.1	1.2	1.5	1.1	1.2	1.4	1.2	0.0	1.1	1.5	1.6	1.7	1.7	1.6	1.4	1.3	1.4	1.8	1.9	1.5
SER	53	27	19	33	29	26	28	0	21	28	54	65	13	36	36	49	49	22	55	75
SER	1.3	1.5	1.5	1.4	1.5	1.4	1.4	0.0	1.5	1.6	1.6	1.7	1.8	1.5	1.5	1.3	1.6	2.3	1.9	1.7
THR	42	21	32	33	16	12	19	0	9	30	59	41	19	26	25	27	27	14	28	40
THR	1.3	1.6	1.3	1.3	1.4	1.8	1.9	0.0	1.2	1.7	1.6	1.6	1.8	1.9	1.7	1.4	1.4	1.4	1.6	1.5
TRP	12	4	6	4	2	7	6	0	3	11	21	7	3	12	9	5	10	6	11	24
TRP	1.4	1.5	1.3	1.0	1.0	1.4	1.0	0.0	1.0	1.8	1.6	1.4	2.3	2.2	2.4	1.0	1.4	2.2	2.3	1.3
TYR	25	15	19	13	8	15	14	0	11	30	33	14	17	18	30	22	16	15	25	31
TYR	1.2	1.4	1.4	1.5	1.8	1.3	1.0	0.0	1.1	1.8	1.8	1.4	2.0	1.7	1.8	1.5	1.8	1.5	1.6	1.3
VAL	55	15	14	18	20	19	29	0	11	37	78	32	10	39	28	40	37	28	32	89
VAL	1.2	1.4	1.4	1.6	1.6	1.7	1.5	0.0	1.5	1.5	1.5	1.4	1.5	1.6	1.6	1.2	1.8	1.6	1.7	1.6

Table 60: Total number of residue-residue interactions and average atom contacts for interactions between secondary structures for backbone atoms and hydrophobic side-chain atoms.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	38	7	5	5	9	8	8	0	7	70	51	12	21	31	3	19	29	18	23	77
ALA	1.6	2.0	1.2	1.2	1.6	1.0	1.8	0.0	1.4	1.5	1.6	1.9	2.1	2.0	1.3	1.2	1.4	1.9	2.3	1.4
ARG	6	4	0	3	2	3	1	0	6	13	11	3	6	14	1	3	5	9	6	14
ARG	1.3	2.5	0.0	2.3	1.0	1.0	1.0	0.0	1.5	1.5	1.8	2.3	1.5	2.0	2.0	1.0	1.4	1.6	2.5	1.4
ASN	3	5	2	6	5	1	2	0	2	10	10	6	4	4	4	2	0	5	9	7
ASN	1.0	1.4	1.0	1.3	1.6	1.0	1.0	0.0	1.0	1.0	1.9	1.2	1.0	1.8	2.0	1.0	0.0	2.8	1.8	1.9
ASP	6	7	1	1	2	5	1	0	3	8	17	9	7	14	3	5	5	7	11	7
ASP	1.3	1.4	1.0	1.0	1.5	1.0	1.0	0.0	1.3	1.5	1.6	2.1	1.1	2.1	1.0	1.0	2.0	2.3	1.5	1.9
CYS	3	2	1	0	31	1	0	0	5	5	18	1	4	3	2	2	4	3	4	12
CYS	1.0	1.0	1.0	0.0	1.6	2.0	0.0	0.0	1.4	1.8	1.4	1.0	1.2	1.3	1.5	1.5	1.0	1.7	1.5	1.5
GLN	4	0	1	6	4	3	1	0	3	7	10	3	4	7	3	3	6	5	5	20
GLN	1.5	0.0	1.0	1.2	1.0	1.3	1.0	0.0	1.0	1.4	1.7	1.0	2.0	1.7	1.7	1.0	1.3	1.4	1.6	1.6
GLU	7	4	2	3	3	0	4	0	0	15	14	6	6	12	2	6	7	4	12	8
GLU	1.4	1.2	1.5	1.3	2.0	0.0	1.8	0.0	0.0	1.5	1.6	1.2	1.5	1.5	1.5	1.7	1.0	2.8	2.1	1.5
GLY	35	7	13	14	10	7	9	0	11	50	72	11	18	33	12	16	29	17	37	62
GLY	1.5	2.1	1.5	1.8	1.6	1.3	2.1	0.0	1.4	2.2	2.1	1.6	2.3	2.8	2.3	1.7	1.3	3.1	2.8	1.9
HIS	6	2	1	1	3	1	0	0	0	6	8	0	2	7	1	8	8	2	4	7
HIS	1.5	1.0	1.0	1.0	1.7	2.0	0.0	0.0	0.0	1.2	1.2	0.0	1.0	2.7	2.0	1.1	1.8	4.5	1.2	1.1
ILE	13	5	5	3	4	3	6	0	7	18	34	9	7	28	0	13	11	10	29	24
ILE	1.2	1.2	1.0	1.0	1.2	1.3	1.3	0.0	1.3	1.3	1.1	1.1	1.4	1.8	0.0	1.0	1.7	1.7	1.7	1.5
LEU	16	8	10	6	5	9	5	0	9	42	47	12	19	36	8	12	14	18	26	30
LEU	1.6	1.6	1.5	1.0	1.2	1.1	1.4	0.0	1.8	1.3	1.4	2.0	1.6	1.8	1.1	1.8	1.6	1.9	1.8	1.3
LYS	8	3	0	6	5	0	5	0	2	15	26	8	11	9	5	10	7	7	8	13
LYS	1.1	1.0	0.0	1.5	1.0	0.0	1.2	0.0	2.0	1.6	1.8	1.8	1.7	2.6	1.6	1.3	1.1	1.7	2.0	1.5
MET	6	11	1	0	6	4	2	0	2	9	7	5	3	8	0	3	7	4	0	12
MET	1.5	1.9	1.0	0.0	1.8	2.2	1.0	0.0	1.0	1.4	1.3	1.4	1.0	1.9	0.0	1.0	1.3	1.5	0.0	1.3
PHE	12	2	3	1	11	3	2	0	3	10	28	10	5	16	3	9	6	7	11	17
PHE	1.2	2.5	1.0	1.0	1.5	1.7	1.5	0.0	1.0	1.1	1.3	1.3	2.4	1.6	1.7	1.1	1.7	1.1	1.5	1.3
PRO	10	5	0	1	4	1	2	0	3	7	21	2	5	6	1	6	6	3	6	20
PRO	1.3	1.8	0.0	1.0	1.2	1.0	1.0	0.0	1.0	1.3	1.2	1.5	1.6	1.5	1.0	1.3	1.2	1.3	1.7	1.3
SER	20	10	4	4	4	4	5	0	5	12	23	12	11	20	6	17	12	14	14	33
SER	1.5	1.8	1.0	1.2	2.0	1.5	1.0	0.0	1.0	1.4	1.4	1.3	1.2	1.5	1.3	1.3	1.7	2.4	2.3	1.5
THR	13	9	3	14	5	5	3	0	5	24	29	11	6	14	5	12	12	9	11	16
THR	1.4	1.3	1.3	1.5	2.2	1.2	1.0	0.0	1.4	1.6	1.8	1.8	1.7	1.4	1.6	1.2	1.5	1.7	1.5	1.2
TRP	5	3	0	1	0	2	3	0	0	7	8	1	2	2	1	3	4	3	5	6
TRP	1.2	1.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	1.3	1.1	1.0	2.5	2.0	2.0	1.0	1.5	1.7	1.6	1.3
TYR	10	3	4	2	6	2	5	0	7	17	16	2	7	11	6	6	12	11	9	15
TYR	1.3	1.7	1.5	2.5	1.7	1.5	1.4	0.0	1.1	1.9	1.4	1.0	2.3	1.4	1.5	1.2	1.8	1.7	1.9	1.2
VAL	26	7	8	6	11	4	11	0	5	23	44	8	10	18	14	19	21	10	16	60
VAL	1.1	1.1	1.0	1.5	1.5	1.5	1.3	0.0	2.0	1.4	1.2	1.5	1.8	1.8	1.2	1.3	1.6	1.6	1.9	1.6

Table 61: Number of residue-residue interactions and average atom contacts for interactions between backbone atoms and hydrophobic side-chain atoms. Interactions are between pairs of α -helices.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	22	2	4	2	3	1	0	0	3	22	26	5	11	15	0	7	6	4	5	24
ALA	1.8	2.5	1.0	1.5	1.3	1.0	0.0	0.0	1.7	1.8	1.7	2.2	1.9	2.2	0.0	1.0	1.5	1.5	3.0	1.4
ARG	2	4	0	1	2	1	0	0	1	4	3	0	3	2	1	0	0	2	2	1
ARG	2.0	2.5	0.0	1.0	1.0	1.0	0.0	0.0	1.0	1.8	2.7	0.0	1.7	1.5	2.0	0.0	0.0	1.0	4.0	2.0
ASN	2	1	0	3	0	1	0	0	1	1	0	4	0	3	3	2	0	0	3	0
ASN	1.0	1.0	0.0	1.3	0.0	1.0	0.0	0.0	1.0	1.0	0.0	1.2	0.0	1.7	2.0	1.0	0.0	0.0	1.3	0.0
ASP	2	1	0	0	0	1	1	0	0	3	2	1	2	4	0	3	2	0	4	1
ASP	1.0	1.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	1.3	1.0	1.0	1.5	2.0	0.0	1.0	2.5	0.0	1.0	3.0
CYS	3	0	0	0	6	0	0	0	2	2	6	0	2	1	1	0	0	0	0	0
CYS	1.0	0.0	0.0	0.0	2.2	0.0	0.0	0.0	1.5	2.0	1.7	0.0	1.0	1.0	2.0	0.0	0.0	0.0	0.0	0.0
GLN	3	0	0	1	0	0	0	0	1	0	0	0	1	0	1	0	0	2	1	1
GLN	1.7	0.0	0.0	2.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	2.0	0.0	2.0	0.0	0.0	1.5	1.0	1.0
GLU	5	1	0	1	0	0	0	0	0	5	5	1	3	3	0	1	1	0	3	6
GLU	1.8	2.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.4	1.6	2.0	1.3	2.0	0.0	3.0	1.0	0.0	2.7	1.7
GLY	11	2	1	4	0	0	6	0	4	8	20	4	4	6	2	5	2	2	7	14
GLY	1.4	3.5	2.0	1.8	0.0	0.0	2.0	0.0	1.8	2.0	2.1	2.5	2.0	2.5	2.0	1.8	2.0	2.0	2.4	1.8
HIS	3	0	0	0	0	0	0	0	0	0	0	2	0	0	1	0	2	4	0	1
HIS	1.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	6.0	0.0	1.5	1.2	0.0	1.0	1.0
ILE	5	1	0	0	0	1	2	0	0	3	5	0	0	2	0	2	1	2	3	4
ILE	1.2	1.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	1.3	1.0	0.0	0.0	2.0	0.0	1.0	1.0	1.0	1.0	1.8
LEU	8	7	0	2	1	2	0	0	2	12	19	6	5	9	3	5	2	4	5	6
LEU	1.9	1.7	0.0	1.0	1.0	1.0	0.0	0.0	1.5	1.6	1.5	2.7	1.4	2.3	1.3	2.4	1.0	1.5	1.6	1.3
LYS	4	0	0	1	0	0	1	0	0	5	6	4	1	1	2	0	1	0	1	0
LYS	1.2	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.4	1.3	2.2	2.0	3.0	2.0	0.0	1.0	0.0	1.0	0.0
MET	3	3	0	0	2	1	0	0	0	1	2	3	1	2	0	0	0	0	0	3
MET	2.0	1.3	0.0	0.0	3.0	4.0	0.0	0.0	0.0	1.0	2.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	1.7
PHE	3	1	0	0	2	0	1	0	0	3	9	4	3	5	0	1	0	1	3	2
PHE	1.7	2.0	0.0	0.0	2.0	0.0	2.0	0.0	0.0	1.0	1.1	1.0	1.7	2.2	0.0	1.0	0.0	1.0	1.3	2.0
PRO	0	2	0	1	0	0	0	0	0	0	8	0	2	2	1	1	3	1	2	7
PRO	0.0	2.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.1	0.0	1.0	2.0	1.0	1.0	1.3	1.0	1.0	1.1
SER	8	6	0	1	3	0	1	0	3	5	10	2	2	2	4	2	1	1	0	4
SER	1.2	2.2	0.0	2.0	2.0	0.0	1.0	0.0	1.0	1.8	1.5	2.0	1.5	1.0	1.5	1.0	2.0	1.0	0.0	1.0
THR	3	2	1	1	0	0	0	0	0	0	5	1	2	1	2	0	0	0	0	2
THR	1.7	1.5	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	2.6	1.0	1.5	1.0	1.5	0.0	0.0	0.0	0.0	1.5
TRP	1	2	0	0	0	1	0	0	0	1	2	0	0	0	0	0	0	0	1	1
TRP	2.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	2.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0
TYR	5	1	1	0	0	0	0	0	1	6	2	0	1	3	4	0	2	4	1	1
TYR	1.4	2.0	2.0	0.0	0.0	0.0	0.0	0.0	1.0	3.2	1.5	0.0	1.0	1.3	1.8	0.0	1.5	1.2	5.0	1.0
VAL	11	1	3	3	0	1	1	0	2	4	9	4	2	4	9	2	1	2	2	9
VAL	1.1	1.0	1.0	2.0	0.0	2.0	1.0	0.0	2.0	1.2	1.3	2.0	2.0	3.2	1.3	1.0	1.0	1.5	1.0	1.4

Table 62: Number of residue-residue interactions and average atom contacts for interactions between backbone atoms and hydrophobic side-chain atoms. Interactions are between α -helices and β -sheets.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	5	0	0	1	0	0	1	0	0	13	7	3	3	4	2	1	4	2	3	23
ALA	1.8	0.0	0.0	1.0	0.0	0.0	3.0	0.0	0.0	1.4	1.6	2.0	1.3	1.0	1.5	2.0	2.2	1.0	6.0	1.8
ARG	0	0	0	0	0	0	0	0	0	2	1	0	0	1	0	0	0	1	0	2
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	2.0	0.0	0.0	0.0	3.0	0.0	1.0
ASN	1	0	0	0	3	0	0	0	0	0	2	1	1	0	0	0	0	2	0	1
ASN	1.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	0.0	0.0	3.5	1.0	1.0	0.0	0.0	0.0	0.0	1.5	0.0	1.0
ASP	0	0	0	1	0	0	0	0	0	0	2	1	2	0	1	0	0	1	0	2
ASP	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	2.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0
CYS	0	0	0	0	10	0	0	0	1	0	2	0	0	0	0	0	0	0	2	1
CYS	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	2.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	1.0
GLN	0	0	0	0	0	0	0	0	0	1	1	1	0	1	1	0	0	0	1	5
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	1.0	0.0	2.0	2.0	0.0	0.0	0.0	2.0	1.8
GLU	0	1	0	0	0	0	0	0	0	4	2	0	0	0	0	1	0	2	0	1
GLU	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.5	0.0	0.0	0.0	0.0	1.0	0.0	1.5	0.0	1.0
GLY	1	2	3	3	0	0	0	0	2	9	6	1	1	2	4	1	2	1	3	9
GLY	2.0	1.0	1.7	2.3	0.0	0.0	0.0	0.0	1.5	1.4	1.7	1.0	2.0	2.5	2.5	2.0	1.5	8.0	1.7	1.8
HIS	0	0	0	0	0	0	0	0	0	2	1	0	0	1	0	3	0	1	0	1
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	1.0	0.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	2.0
ILE	0	0	2	0	0	0	0	0	0	4	4	2	1	3	0	0	0	0	1	4
ILE	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	1.2	1.5	1.0	2.0	0.0	0.0	0.0	0.0	2.0	1.8
LEU	0	0	2	0	0	0	0	0	0	5	7	2	2	0	0	0	1	0	4	3
LEU	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.4	1.9	1.5	1.5	0.0	0.0	0.0	2.0	0.0	1.8	1.3
LYS	0	1	0	0	1	0	0	0	0	2	5	0	2	2	0	2	0	0	0	2
LYS	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.5	2.0	0.0	2.0	3.0	0.0	2.0	0.0	0.0	0.0	2.0
MET	0	0	0	0	3	0	0	0	0	3	1	0	0	0	0	0	0	1	0	0
MET	0.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	0.0	1.3	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
PHE	0	1	0	0	1	1	0	0	0	3	0	0	0	3	0	1	0	1	1	1
PHE	0.0	3.0	0.0	0.0	2.0	1.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	1.3	0.0	1.0	0.0	1.0	2.0	1.0
PRO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0
SER	1	0	0	0	0	0	0	0	0	1	1	1	1	2	0	3	1	1	4	11
SER	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0	5.0	5.0	3.5	1.3
THR	2	1	0	0	1	0	0	0	1	2	1	1	0	2	1	0	0	1	0	3
THR	2.0	2.0	0.0	0.0	4.0	0.0	0.0	0.0	1.0	2.0	2.0	3.0	0.0	1.0	2.0	0.0	0.0	3.0	0.0	1.3
TRP	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
TRP	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	1	0	0	0	0	0	2	0	1	0	2	0	0	0	0	1	0	0
TYR	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	3.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
VAL	0	0	0	0	0	0	0	0	2	1	5	0	0	0	2	0	0	0	1	1
VAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0	1.0	1.0

Table 63: Number of residue-residue interactions and average atom contacts for interactions between backbone atoms and hydrophobic side-chain atoms. Interactions are between β -sheets and α -helices.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	5	1	0	0	4	1	0	0	1	7	1	1	0	3	0	5	9	0	0	2
ALA	1.8	2.0	0.0	0.0	2.0	1.0	0.0	0.0	1.0	1.4	1.0	1.0	0.0	1.3	0.0	1.4	1.3	0.0	0.0	1.5
ARG	1	0	0	0	0	0	0	0	1	2	2	0	0	1	0	0	0	1	0	1
ARG	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.0	1.5	0.0	0.0	3.0	0.0	0.0	0.0	1.0	0.0	2.0
ASN	0	1	1	1	0	0	0	0	1	2	0	0	1	0	0	0	0	2	0	0
ASN	0.0	1.0	1.0	2.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0
ASP	2	0	0	0	2	1	0	0	0	1	4	2	0	1	0	0	0	3	0	0
ASP	2.0	0.0	0.0	0.0	1.5	1.0	0.0	0.0	0.0	1.0	1.0	3.0	0.0	2.0	0.0	0.0	0.0	3.7	0.0	0.0
CYS	0	1	0	0	8	0	0	0	0	1	0	0	2	0	1	0	1	1	0	0
CYS	0.0	1.0	0.0	0.0	1.2	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.5	0.0	1.0	0.0	1.0	1.0	0.0	0.0
GLN	0	0	0	0	0	2	0	0	0	0	1	1	1	0	1	0	0	0	0	4
GLN	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	2.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	1.5
GLU	0	0	0	0	1	0	1	0	0	1	1	2	1	1	1	0	2	0	0	0
GLU	0.0	0.0	0.0	0.0	3.0	0.0	1.0	0.0	0.0	6.0	1.0	1.0	2.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0
GLY	11	1	1	2	3	0	1	0	1	11	13	1	4	6	1	2	9	3	3	8
GLY	1.8	1.0	1.0	1.5	2.0	0.0	2.0	0.0	1.0	2.9	2.1	1.0	1.5	2.5	1.0	1.5	1.2	2.0	1.3	2.1
HIS	0	0	0	0	0	0	0	0	0	1	0	0	1	1	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	1	2	0	1	1	1	1	0	4	2	1	1	2	4	0	1	1	3	1	1
ILE	1.0	1.0	0.0	1.0	1.0	1.0	3.0	0.0	1.5	1.0	1.0	1.0	1.0	1.2	0.0	1.0	1.0	2.3	2.0	3.0
LEU	1	1	0	0	0	0	1	0	2	8	0	1	4	8	0	1	2	2	1	2
LEU	3.0	1.0	0.0	0.0	0.0	0.0	2.0	0.0	1.5	1.0	0.0	1.0	1.5	2.5	0.0	3.0	2.0	1.0	2.0	2.0
LYS	0	0	0	0	0	0	0	0	0	1	4	1	4	1	0	0	0	1	0	1
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.5	1.0	1.8	4.0	0.0	0.0	0.0	1.0	0.0	1.0
MET	1	2	1	0	0	2	0	0	2	1	1	0	1	0	0	0	2	1	0	0
MET	1.0	2.0	1.0	0.0	0.0	2.0	0.0	0.0	1.0	3.0	1.0	0.0	1.0	0.0	0.0	0.0	1.5	2.0	0.0	0.0
PHE	1	0	0	0	4	0	0	0	0	0	2	1	1	0	1	2	0	3	1	2
PHE	1.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0	2.0	1.0	4.0	0.0	1.0	1.0	0.0	1.0	1.0	1.5
PRO	4	1	0	0	1	0	0	0	3	3	1	0	0	2	0	0	0	1	0	0
PRO	1.2	1.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	1.3	1.0	0.0	0.0	1.5	0.0	0.0	0.0	1.0	0.0	0.0
SER	1	1	2	0	0	2	1	0	0	2	0	0	1	3	0	2	3	4	0	3
SER	3.0	2.0	1.0	0.0	0.0	2.0	1.0	0.0	0.0	1.5	0.0	0.0	1.0	1.7	0.0	1.5	1.7	2.0	0.0	2.3
THR	1	0	0	5	2	1	0	0	4	3	6	3	2	3	0	1	4	2	1	0
THR	2.0	0.0	0.0	1.4	2.0	1.0	0.0	0.0	1.5	1.3	2.0	1.3	2.5	1.3	0.0	1.0	1.5	1.5	2.0	0.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0
TYR	1	0	1	0	4	0	0	0	1	0	0	0	0	0	0	1	1	0	0	2
TYR	2.0	0.0	1.0	0.0	2.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	3.0	0.0	0.0	1.5
VAL	1	0	1	1	2	0	0	0	1	2	4	0	1	3	0	3	5	1	0	7
VAL	1.0	0.0	1.0	1.0	1.5	0.0	0.0	0.0	2.0	1.0	1.2	0.0	1.0	1.0	0.0	2.0	1.6	1.0	0.0	2.1

Table 64: Number of residue-residue interactions and average atom contacts for interactions between backbone atoms and hydrophobic side-chain atoms. Interactions are between pairs of β -sheets.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	6	4	1	2	2	6	7	0	3	28	17	3	7	9	1	6	10	12	15	28
ALA	1.5	1.8	2.0	1.0	1.0	1.0	1.6	0.0	1.3	1.4	1.5	1.7	2.7	2.3	1.0	1.0	1.0	2.2	1.3	1.3
ARG	3	0	0	2	0	2	1	0	4	5	5	3	3	10	0	3	5	5	4	10
ARG	1.0	0.0	0.0	3.0	0.0	1.0	1.0	0.0	1.8	1.2	1.6	2.3	1.3	2.0	0.0	1.0	1.4	1.6	1.8	1.3
ASN	0	3	1	2	2	0	2	0	0	7	8	1	2	1	1	0	0	1	6	6
ASN	0.0	1.7	1.0	1.0	2.0	0.0	1.0	0.0	0.0	1.0	1.5	1.0	1.0	2.0	2.0	0.0	0.0	3.0	2.0	2.0
ASP	2	6	1	0	0	3	0	0	3	4	9	5	3	9	2	2	3	3	7	4
ASP	1.0	1.5	1.0	0.0	0.0	1.0	0.0	0.0	1.3	1.8	1.8	2.0	1.0	2.2	1.0	1.0	1.7	1.3	1.7	2.0
CYS	0	1	1	0	7	1	0	0	2	2	10	1	0	2	0	2	3	2	2	11
CYS	0.0	1.0	1.0	0.0	1.1	2.0	0.0	0.0	1.0	2.0	1.3	1.0	0.0	1.5	0.0	1.5	1.0	2.0	1.5	1.5
GLN	1	0	1	5	4	1	1	0	2	6	8	1	2	6	0	3	6	3	3	10
GLN	1.0	0.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.3	1.6	1.0	2.5	1.7	0.0	1.0	1.3	1.3	1.7	1.6
GLU	2	2	2	2	2	0	3	0	0	5	6	3	2	8	1	4	4	2	9	1
GLU	1.0	1.0	1.5	1.5	1.5	0.0	2.0	0.0	0.0	1.0	1.3	1.0	1.5	1.4	2.0	1.5	1.0	4.0	1.9	1.0
GLY	12	2	8	5	7	7	2	0	4	22	33	5	9	19	5	8	16	11	24	31
GLY	1.3	2.5	1.5	1.6	1.4	1.3	2.5	0.0	1.0	2.3	2.1	1.2	2.9	3.1	2.6	1.6	1.2	3.1	3.0	2.0
HIS	3	2	1	1	3	1	0	0	0	3	5	0	1	4	1	3	4	1	3	5
HIS	1.3	1.0	1.0	1.0	1.7	2.0	0.0	0.0	0.0	1.0	1.4	0.0	1.0	2.5	2.0	1.0	2.2	8.0	1.3	1.0
ILE	7	2	3	2	3	1	3	0	3	9	24	6	4	17	0	10	9	5	24	15
ILE	1.3	1.5	1.0	1.0	1.3	2.0	1.0	0.0	1.0	1.3	1.2	1.0	1.8	1.9	0.0	1.0	1.9	1.6	1.8	1.3
LEU	7	0	8	4	4	7	4	0	5	19	21	3	8	21	5	6	9	12	16	19
LEU	1.1	0.0	1.6	1.0	1.2	1.1	1.2	0.0	2.0	1.2	1.2	1.3	1.9	1.4	1.0	1.0	1.7	2.2	1.8	1.3
LYS	4	2	0	5	4	0	4	0	2	7	11	3	4	5	3	8	6	6	7	10
LYS	1.0	1.0	0.0	1.6	1.0	0.0	1.2	0.0	2.0	1.7	2.1	1.3	1.5	2.0	1.3	1.1	1.2	1.8	2.1	1.4
MET	2	6	0	0	1	1	2	0	0	4	3	2	1	6	0	3	5	2	0	9
MET	1.0	2.2	0.0	0.0	1.0	1.0	1.0	0.0	0.0	1.2	1.0	2.0	1.0	2.2	0.0	1.0	1.2	1.5	0.0	1.2
PHE	8	0	3	1	4	2	1	0	3	4	17	5	1	8	2	5	6	2	6	12
PHE	1.0	0.0	1.0	1.0	1.0	2.0	1.0	0.0	1.0	1.0	1.4	1.6	3.0	1.2	2.0	1.2	1.7	1.5	1.7	1.2
PRO	6	2	0	0	3	1	2	0	0	4	12	2	3	2	0	5	3	1	4	12
PRO	1.3	2.0	0.0	0.0	1.3	1.0	1.0	0.0	0.0	1.2	1.3	1.5	2.0	1.0	0.0	1.4	1.0	2.0	2.0	1.3
SER	10	3	2	3	1	2	3	0	2	4	12	9	7	13	2	10	7	8	10	15
SER	1.6	1.0	1.0	1.0	2.0	1.0	1.0	0.0	1.0	1.0	1.3	1.2	1.1	1.5	1.0	1.4	1.1	2.5	1.8	1.7
THR	7	6	2	8	2	4	3	0	0	19	17	6	2	8	2	11	8	6	10	11
THR	1.0	1.2	1.5	1.6	1.5	1.2	1.0	0.0	0.0	1.6	1.5	2.0	1.0	1.6	1.5	1.3	1.5	1.5	1.4	1.2
TRP	3	1	0	1	0	1	3	0	0	6	6	1	1	2	1	3	3	3	4	5
TRP	1.0	1.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	1.2	1.0	1.0	2.0	2.0	2.0	1.0	1.0	1.7	1.5	1.2
TYR	4	2	1	2	2	2	5	0	3	11	13	2	4	8	2	5	9	6	8	12
TYR	1.0	1.5	1.0	2.5	1.0	1.5	1.4	0.0	1.0	1.3	1.5	1.0	2.2	1.4	1.0	1.0	1.8	2.2	1.5	1.2
VAL	14	6	4	2	9	3	10	0	0	16	26	4	7	11	3	14	15	7	13	43
VAL	1.1	1.2	1.0	1.0	1.6	1.3	1.3	0.0	0.0	1.5	1.2	1.0	1.9	1.5	1.0	1.1	1.7	1.7	2.1	1.5

APPENDIX H

Table 65: Total number of residue-residue interactions and average atom contacts for interactions between hydrophobic side-chain atoms.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	154	30	34	51	22	50	32	0	35	246	307	72	74	159	58	76	96	62	142	295
ALA	1.0	1.4	1.3	1.3	1.1	1.3	1.3	NaN	1.2	1.4	1.3	1.3	1.6	2.0	1.6	1.0	1.2	2.0	2.3	1.2
ARG	30	38	25	41	10	23	56	0	15	74	92	21	18	52	35	31	32	37	73	79
ARG	1.4	2.6	1.9	1.6	1.7	1.9	1.8	NaN	2.5	2.4	1.8	2.1	2.2	3.5	2.1	1.6	2.0	4.4	3.1	2.0
ASN	34	25	12	44	6	18	45	0	19	42	54	46	26	42	15	15	35	35	52	64
ASN	1.3	1.9	1.2	1.3	1.5	1.4	1.5	NaN	1.6	1.5	1.5	1.9	1.9	2.2	1.6	1.3	1.4	2.7	2.1	1.4
ASP	51	41	44	10	15	22	30	0	33	68	75	93	9	50	29	52	58	18	64	56
ASP	1.3	1.8	1.3	1.4	1.4	1.4	1.4	NaN	1.3	1.5	1.7	1.8	1.3	2.2	1.7	1.2	1.3	2.3	2.0	1.4
CYS	22	10	6	15	172	18	18	0	20	47	98	17	33	59	36	35	25	14	48	87
CYS	1.1	1.7	1.5	1.4	4.0	2.1	1.6	NaN	1.9	1.9	2.0	2.2	2.2	2.5	1.7	1.1	1.5	1.9	2.7	1.6
GLN	50	23	16	22	18	22	20	0	12	58	84	36	14	44	40	23	32	31	49	77
GLN	1.3	1.9	1.4	1.4	2.1	1.8	1.6	NaN	1.8	1.7	2.1	1.8	1.9	3.0	1.8	1.4	1.3	2.8	3.2	1.6
GLU	32	56	45	30	16	20	22	0	32	74	92	111	27	60	33	47	48	27	51	83
GLU	1.3	1.8	1.5	1.4	1.6	1.6	1.5	NaN	1.7	2.0	1.9	2.0	2.1	2.8	1.7	1.2	1.5	2.4	2.8	1.9
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN
HIS	35	15	19	33	20	12	32	0	42	51	75	23	25	60	31	40	39	37	66	62
HIS	1.2	2.5	1.6	1.3	1.9	1.8	1.7	NaN	1.3	2.2	2.6	2.8	2.6	3.3	2.7	1.3	2.2	3.9	3.1	1.7
ILE	246	74	42	68	47	58	74	0	51	390	527	102	103	252	70	62	125	119	167	388
ILE	1.4	2.4	1.5	1.5	1.9	1.7	2.0	NaN	2.2	2.0	1.9	2.2	2.0	2.9	2.0	1.1	1.7	3.3	3.0	1.8
LEU	307	92	54	75	98	84	92	0	75	527	900	129	162	449	137	99	169	152	208	727
LEU	1.3	1.8	1.5	1.7	2.0	2.1	1.9	NaN	2.6	1.9	1.8	2.1	2.0	2.6	1.8	1.3	1.7	3.3	3.0	1.7
LYS	72	21	48	93	17	36	111	0	23	102	129	40	35	75	48	70	62	51	98	117
LYS	1.3	2.1	1.9	1.8	2.2	1.8	2.0	NaN	2.8	2.2	2.1	2.3	2.3	4.4	2.4	1.6	1.8	5.4	4.1	2.0
MET	74	18	26	9	33	14	27	0	25	103	162	35	36	94	34	33	29	36	67	100
MET	1.6	2.2	1.9	1.3	2.2	1.9	2.1	NaN	2.6	2.0	2.0	2.3	2.3	3.2	2.1	1.4	2.0	3.4	2.8	2.0
PHE	159	52	42	50	59	44	60	0	60	252	449	75	94	282	72	67	90	91	134	337
PHE	2.0	3.5	2.2	2.2	2.5	3.0	2.8	NaN	3.3	2.9	2.6	4.4	3.2	3.6	4.1	1.8	2.3	4.2	3.1	2.5
PRO	58	35	15	29	36	40	33	0	31	70	137	48	34	72	46	29	64	64	110	128
PRO	1.8	2.1	1.6	1.7	1.7	1.8	1.7	NaN	2.7	2.0	1.8	2.4	2.1	4.1	2.2	1.6	2.0	4.3	4.2	1.9
SER	76	31	15	52	35	23	47	0	40	62	99	70	33	67	29	44	78	24	87	113
SER	1.0	1.6	1.3	1.2	1.1	1.4	1.2	NaN	1.3	1.1	1.3	1.6	1.4	1.8	1.6	1.0	1.2	1.9	1.9	1.3
THR	96	32	35	58	25	32	48	0	39	125	169	62	29	90	64	78	78	32	85	130
THR	1.2	2.0	1.4	1.3	1.5	1.3	1.5	NaN	2.2	1.7	1.7	1.8	2.0	2.3	2.0	1.2	1.4	2.2	2.2	1.5
TRP	62	37	35	18	14	31	27	0	37	119	152	51	36	91	64	24	32	60	48	116
TRP	2.0	4.4	2.7	2.3	1.9	2.8	2.4	NaN	3.9	3.3	3.3	5.4	3.4	4.2	4.3	1.9	2.2	4.5	3.3	3.3
TYR	142	73	52	64	48	49	51	0	66	167	206	98	67	134	110	87	85	48	138	199
TYR	2.3	3.1	2.1	2.0	2.7	3.2	2.8	NaN	3.1	3.0	3.0	4.1	2.8	3.1	4.2	1.9	2.2	3.3	3.4	2.7
VAL	295	79	64	56	87	77	83	0	62	388	727	117	100	337	128	113	130	116	199	576
VAL	1.2	2.0	1.4	1.4	1.6	1.6	1.9	NaN	1.7	1.8	1.7	2.0	2.0	2.5	1.9	1.3	1.5	3.3	2.7	1.7

Table 66: Total number of residue-residue interactions and average atom contacts for interactions between secondary structures involving hydrophobic side-chain atoms.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	76	11	8	9	4	14	13	0	12	126	148	20	35	75	17	23	39	29	52	160
ALA	1.0	1.4	1.1	1.4	1.0	1.2	1.5	0.0	1.3	1.3	1.3	1.2	1.6	2.0	1.5	1.0	1.2	2.2	2.1	1.2
ARG	11	6	3	8	4	7	9	0	2	34	35	2	10	16	10	8	8	7	23	25
ARG	1.4	3.7	1.0	2.0	1.8	1.7	2.3	0.0	1.0	2.9	2.1	1.5	2.4	3.2	2.6	2.0	2.0	7.6	3.0	2.1
ASN	8	3	0	6	1	5	6	0	4	16	15	6	8	5	1	4	5	7	11	15
ASN	1.1	1.0	0.0	1.2	1.0	1.4	1.2	0.0	2.0	1.5	1.5	2.5	2.4	2.8	1.0	1.0	1.0	2.0	2.4	1.3
ASP	9	8	6	2	7	3	10	0	6	19	21	13	2	13	2	6	4	5	16	9
ASP	1.4	2.0	1.2	2.0	1.4	1.3	1.5	0.0	1.0	1.5	1.4	1.6	1.5	2.7	1.5	1.2	1.2	1.8	2.1	1.2
CYS	4	4	1	7	40	3	3	0	7	18	38	5	17	21	4	5	8	5	13	17
CYS	1.0	1.8	1.0	1.4	4.0	2.3	1.7	0.0	2.0	1.8	1.8	3.0	2.4	2.3	1.5	1.0	1.8	2.2	2.0	1.4
GLN	14	7	5	3	3	2	4	0	9	16	24	6	5	10	7	6	8	7	13	31
GLN	1.2	1.7	1.4	1.3	2.3	4.0	1.2	0.0	2.0	1.6	1.9	1.7	2.2	3.1	1.4	1.3	1.1	5.1	2.7	1.5
GLU	13	9	6	10	3	4	0	0	6	32	32	28	10	12	7	9	14	7	17	27
GLU	1.5	2.3	1.2	1.5	1.7	1.2	0.0	0.0	1.5	2.0	1.8	2.1	1.9	4.3	1.6	1.3	1.9	3.3	2.9	2.4
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	12	2	4	6	7	9	6	0	18	16	27	2	11	18	5	15	8	7	15	20
HIS	1.3	1.0	2.0	1.0	2.0	2.0	1.5	0.0	1.2	2.2	2.6	1.5	2.5	3.5	3.6	1.7	2.5	3.7	4.8	1.9
ILE	126	34	16	19	18	16	32	0	16	148	236	37	32	97	22	20	36	39	57	156
ILE	1.3	2.9	1.5	1.5	1.8	1.6	2.0	0.0	2.2	2.1	1.9	2.4	2.1	2.8	2.2	1.1	1.8	3.4	2.5	1.8
LEU	148	35	15	21	38	24	32	0	27	236	456	31	67	180	35	19	73	58	75	296
LEU	1.3	2.1	1.5	1.4	1.8	1.9	1.8	0.0	2.6	1.9	1.8	2.0	2.1	2.6	1.5	1.4	1.7	3.6	3.1	1.7
LYS	20	2	6	13	5	6	28	0	2	37	31	4	11	16	5	13	18	17	16	38
LYS	1.2	1.5	2.5	1.6	3.0	1.7	2.1	0.0	1.5	2.4	2.0	3.0	1.6	3.9	3.2	1.5	1.7	6.1	4.6	2.0
MET	35	10	8	2	17	5	10	0	11	32	67	11	10	42	9	6	11	14	11	48
MET	1.6	2.4	2.4	1.5	2.4	2.2	1.9	0.0	2.5	2.1	2.1	1.6	1.4	3.3	2.6	1.5	2.7	3.6	3.6	2.0
PHE	75	16	5	13	21	10	12	0	18	97	180	16	42	140	9	20	28	32	43	136
PHE	2.0	3.2	2.8	2.7	2.3	3.1	4.3	0.0	3.5	2.8	2.8	3.9	3.3	3.5	3.9	2.5	2.4	4.9	3.3	2.5
PRO	17	10	1	2	4	7	7	0	5	22	35	5	9	9	0	5	14	16	8	32
PRO	1.5	2.6	1.0	1.5	1.5	1.4	1.6	0.0	3.6	2.2	1.5	3.2	2.6	3.9	0.0	1.6	2.2	3.7	3.4	1.9
SER	23	8	4	6	5	6	9	0	15	20	19	13	6	20	5	10	16	3	17	37
SER	1.0	2.0	1.0	1.2	1.0	1.3	1.3	0.0	1.7	1.1	1.4	1.5	1.5	2.5	1.6	1.0	1.1	1.7	1.9	1.3
THR	39	8	5	4	8	8	14	0	8	36	73	18	11	28	14	16	20	5	24	38
THR	1.2	2.0	1.0	1.2	1.8	1.1	1.9	0.0	2.5	1.8	1.7	1.7	2.7	2.4	2.2	1.1	1.3	2.2	2.2	1.5
TRP	29	7	7	5	5	7	7	0	7	39	58	17	14	32	16	3	5	20	18	35
TRP	2.2	7.6	2.0	1.8	2.2	5.1	3.3	0.0	3.7	3.4	3.6	6.1	3.6	4.9	3.7	1.7	2.2	5.5	3.1	3.3
TYR	52	23	11	16	13	13	17	0	15	57	75	16	11	43	8	17	24	18	36	66
TYR	2.1	3.0	2.4	2.1	2.0	2.7	2.9	0.0	4.6	2.5	3.1	4.6	3.6	3.3	3.4	1.9	2.2	3.1	4.1	2.7
VAL	160	25	15	9	17	31	27	0	20	156	296	38	48	136	32	37	38	35	66	302
VAL	1.2	2.1	1.3	1.2	1.4	1.5	2.4	0.0	1.9	1.8	1.7	2.0	2.0	2.5	1.9	1.3	1.5	3.3	2.7	1.8

Table 67: Number of residue-residue interactions and average atom contacts for interactions between hydrophobic side-chain atoms. Interactions are between pairs of α -helices.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	46	9	6	5	1	5	7	0	7	46	75	13	21	34	5	9	11	8	9	61
ALA	1.0	1.3	1.2	1.6	1.0	1.4	1.6	0.0	1.3	1.5	1.3	1.3	1.5	2.1	1.4	1.0	1.4	2.0	3.1	1.2
ARG	9	6	2	3	3	3	3	0	2	14	19	0	4	5	5	6	2	2	9	13
ARG	1.3	3.7	1.0	2.3	1.7	2.0	3.3	0.0	1.0	2.1	1.9	0.0	2.0	3.8	2.6	2.0	2.5	9.5	3.4	2.0
ASN	6	2	0	2	0	1	0	0	4	3	3	4	3	3	1	4	1	1	5	4
ASN	1.2	1.0	0.0	1.0	0.0	1.0	0.0	0.0	2.0	1.0	1.7	2.2	2.7	2.7	1.0	1.0	1.0	1.0	2.0	1.5
ASP	5	3	2	2	1	0	4	0	2	5	6	7	2	7	2	3	1	0	6	2
ASP	1.8	2.3	1.0	2.0	2.0	0.0	1.2	0.0	1.0	1.4	1.8	1.6	1.5	2.6	1.5	1.3	1.0	0.0	2.2	1.0
CYS	1	3	0	1	6	0	1	0	2	7	13	0	6	6	1	1	1	0	2	3
CYS	1.0	1.7	0.0	2.0	4.0	0.0	2.0	0.0	2.0	2.1	1.7	0.0	1.5	2.2	1.0	1.0	2.0	0.0	2.0	1.3
GLN	5	3	1	0	0	0	1	0	4	5	12	1	4	3	0	5	0	2	4	8
GLN	1.4	2.0	1.0	0.0	0.0	0.0	1.0	0.0	1.8	1.8	1.8	1.0	2.0	3.3	0.0	1.2	0.0	6.0	2.5	1.4
GLU	7	3	0	4	1	1	0	0	5	9	17	14	6	6	3	4	5	4	4	14
GLU	1.6	3.3	0.0	1.2	2.0	1.0	0.0	0.0	1.6	2.0	1.9	1.7	1.5	4.8	1.7	1.5	2.2	1.8	5.0	2.3
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	7	2	4	2	2	4	5	0	6	4	15	0	6	11	0	10	4	1	4	9
HIS	1.3	1.0	2.0	1.0	2.0	1.8	1.6	0.0	1.3	3.0	2.5	0.0	2.3	4.5	0.0	1.5	2.5	1.0	8.0	2.0
ILE	46	14	3	5	7	5	9	0	4	22	70	14	7	30	2	7	8	11	17	35
ILE	1.5	2.1	1.0	1.4	2.1	1.8	2.0	0.0	3.0	2.6	1.9	2.2	1.4	3.0	3.0	1.1	1.5	3.6	2.6	1.9
LEU	75	19	3	6	13	12	17	0	15	70	214	11	30	64	14	15	27	25	38	96
LEU	1.3	1.9	1.7	1.8	1.7	1.8	1.9	0.0	2.5	1.9	1.7	1.5	1.9	2.8	1.4	1.4	1.8	3.6	3.0	1.4
LYS	13	0	4	7	0	1	14	0	0	14	11	0	3	4	2	4	0	3	7	15
LYS	1.3	0.0	2.2	1.6	0.0	1.0	1.7	0.0	0.0	2.2	1.5	0.0	2.0	3.0	4.5	1.2	0.0	3.7	4.4	1.9
MET	21	4	3	2	6	4	6	0	6	7	30	3	2	16	3	2	5	5	3	16
MET	1.5	2.0	2.7	1.5	1.5	2.0	1.5	0.0	2.3	1.4	1.9	2.0	2.0	2.8	3.3	1.0	4.0	2.8	2.0	1.9
PHE	34	5	3	7	6	3	6	0	11	30	64	4	16	64	3	4	4	12	12	37
PHE	2.1	3.8	2.7	2.6	2.2	3.3	4.8	0.0	4.5	3.0	2.8	3.0	2.8	3.3	2.3	1.5	2.8	5.8	3.6	2.6
PRO	5	5	1	2	1	0	3	0	0	2	14	2	3	3	0	1	7	6	4	13
PRO	1.4	2.6	1.0	1.5	1.0	0.0	1.7	0.0	0.0	3.0	1.4	4.5	3.3	2.3	0.0	2.0	3.1	3.5	1.5	2.1
SER	9	6	4	3	1	5	4	0	10	7	15	4	2	4	1	0	1	1	7	9
SER	1.0	2.0	1.0	1.3	1.0	1.2	1.5	0.0	1.5	1.1	1.4	1.2	1.0	1.5	2.0	0.0	1.0	2.0	1.7	1.3
THR	11	2	1	1	1	0	5	0	4	8	27	0	5	4	7	1	0	0	4	6
THR	1.4	2.5	1.0	1.0	2.0	0.0	2.2	0.0	2.5	1.5	1.8	0.0	4.0	2.8	3.1	1.0	0.0	0.0	1.8	1.3
TRP	8	2	1	0	0	2	4	0	1	11	25	3	5	12	6	1	0	6	7	9
TRP	2.0	9.5	1.0	0.0	0.0	6.0	1.8	0.0	1.0	3.6	3.6	3.7	2.8	5.8	3.5	2.0	0.0	5.3	2.0	2.7
TYR	9	9	5	6	2	4	4	0	4	17	38	7	3	12	4	7	4	7	12	16
TYR	3.1	3.4	2.0	2.2	2.0	2.5	5.0	0.0	8.0	2.6	3.0	4.4	2.0	3.6	1.5	1.7	1.8	2.0	3.7	3.1
VAL	61	13	4	2	3	8	14	0	9	35	96	15	16	37	13	9	6	9	16	68
VAL	1.2	2.0	1.5	1.0	1.3	1.4	2.3	0.0	2.0	1.9	1.4	1.9	1.9	2.6	2.1	1.3	1.3	2.7	3.1	1.7

Table 68: Number of residue-residue interactions and average atom contacts for interactions between hydrophobic side-chain atoms. Interactions are between α -helices and β -sheets.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	12	1	2	1	0	0	2	0	0	26	25	1	6	15	1	4	9	4	18	42
ALA	1.0	2.0	1.0	2.0	0.0	0.0	1.5	0.0	0.0	1.4	1.3	1.0	2.0	1.8	2.0	1.0	1.1	3.8	1.9	1.2
ARG	0	0	0	2	1	0	0	0	0	10	4	0	4	2	3	0	1	1	0	4
ARG	0.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	0.0	4.1	2.5	0.0	2.8	4.5	2.0	0.0	2.0	12.0	0.0	1.5
ASN	0	1	0	0	1	0	0	0	0	2	1	0	2	2	0	0	0	2	0	1
ASN	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.5	1.0	0.0	2.5	3.0	0.0	0.0	0.0	2.0	0.0	1.0
ASP	0	0	2	0	1	0	0	0	0	0	3	1	0	1	0	1	0	1	1	3
ASP	0.0	0.0	1.5	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.3	1.0	0.0	5.0	0.0	1.0	0.0	1.0	3.0	1.3
CYS	1	0	0	2	11	0	0	0	1	3	8	0	1	3	2	0	4	1	6	4
CYS	1.0	0.0	0.0	1.5	4.0	0.0	0.0	0.0	1.0	2.3	2.4	0.0	1.0	2.0	2.0	0.0	1.8	1.0	1.8	1.0
GLN	2	1	2	0	0	1	0	0	0	3	1	1	0	2	2	1	3	0	2	6
GLN	1.0	1.0	2.0	0.0	0.0	4.0	0.0	0.0	0.0	2.0	1.0	1.0	0.0	3.5	2.0	2.0	1.3	0.0	2.5	1.2
GLU	1	1	1	0	1	0	0	0	1	14	3	2	2	4	0	1	0	1	2	4
GLU	1.0	2.0	2.0	0.0	1.0	0.0	0.0	0.0	1.0	2.2	1.3	1.0	1.5	5.0	0.0	1.0	0.0	9.0	2.0	1.8
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	2	0	0	3	0	0	0	0	0	8	3	0	1	1	4	3	2	2	4	4
HIS	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	2.4	4.7	0.0	1.0	1.0	4.2	3.0	1.5	2.5	5.2	1.5
ILE	12	1	2	0	4	1	0	0	0	29	29	4	5	15	8	1	1	7	9	12
ILE	1.2	2.0	2.0	0.0	1.5	1.0	0.0	0.0	0.0	1.9	1.8	2.5	2.2	3.1	2.2	2.0	1.0	4.6	3.8	2.3
LEU	12	2	1	3	1	0	2	0	2	47	42	2	6	22	5	0	6	5	9	38
LEU	1.2	2.0	1.0	1.0	1.0	0.0	2.0	0.0	2.5	2.0	1.9	1.0	2.8	3.1	2.2	0.0	1.8	4.4	3.8	1.6
LYS	1	0	0	1	1	1	0	0	0	8	9	1	0	1	1	1	1	4	0	8
LYS	1.0	0.0	0.0	1.0	1.0	3.0	0.0	0.0	0.0	2.6	2.2	5.0	0.0	7.0	1.0	1.0	1.0	2.0	0.0	2.5
MET	2	0	2	0	3	1	2	0	0	10	7	2	1	8	0	0	1	1	3	8
MET	1.5	0.0	1.5	0.0	2.7	3.0	3.5	0.0	0.0	2.5	1.7	1.5	2.0	2.6	0.0	0.0	2.0	8.0	3.7	2.6
PHE	6	2	0	0	2	1	0	0	1	12	15	2	1	13	2	4	2	2	5	16
PHE	1.7	1.5	0.0	0.0	2.5	2.0	0.0	0.0	4.0	1.8	2.9	6.0	1.0	3.7	4.5	1.5	2.0	5.5	4.2	2.5
PRO	3	0	0	0	0	1	0	0	1	1	3	0	0	2	0	1	0	0	0	1
PRO	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	1.3	0.0	0.0	3.5	0.0	1.0	0.0	0.0	0.0	2.0
SER	3	0	0	0	0	0	0	0	0	2	0	0	0	3	0	0	1	0	3	10
SER	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	3.0	0.0	0.0	1.0	0.0	1.3	1.3
THR	7	0	0	0	0	0	0	0	0	9	9	1	3	7	2	2	4	1	1	9
THR	1.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.9	1.6	1.0	1.3	2.7	2.0	1.0	1.0	1.0	1.0	2.1
TRP	5	0	3	1	1	1	0	0	0	5	8	2	4	6	3	1	1	2	2	6
TRP	2.6	0.0	2.7	1.0	1.0	11.0	0.0	0.0	0.0	4.8	4.0	11.5	3.0	4.5	3.7	1.0	3.0	4.5	1.0	2.5
TYR	1	1	0	0	0	1	0	0	2	5	3	1	1	6	2	0	2	2	2	2
TYR	1.0	2.0	0.0	0.0	0.0	1.0	0.0	0.0	3.0	2.0	2.0	6.0	3.0	2.7	7.0	0.0	2.0	4.5	8.0	2.0
VAL	12	0	0	0	0	1	0	0	1	23	25	4	3	21	2	5	1	3	11	41
VAL	1.2	0.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0	1.6	1.7	2.5	1.0	2.0	2.5	1.8	1.0	1.3	3.1	1.9

Table 69: Number of residue-residue interactions and average atom contacts for interactions between hydrophobic side-chain atoms. Interactions are between β -sheets and α -helices.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	12	0	0	0	1	2	1	0	2	12	12	1	2	6	3	3	7	5	1	12
ALA	1.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	1.0	1.2	1.2	1.0	1.5	1.7	1.0	1.0	1.1	2.6	1.0	1.2
ARG	1	0	1	0	0	1	1	0	0	1	2	0	0	2	0	0	0	0	1	0
ARG	2.0	0.0	1.0	0.0	0.0	1.0	2.0	0.0	0.0	2.0	2.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	2.0	0.0
ASN	2	0	0	2	0	2	1	0	0	2	1	0	2	0	0	0	0	3	0	0
ASN	1.0	0.0	0.0	1.5	0.0	2.0	2.0	0.0	0.0	2.0	1.0	0.0	1.5	0.0	0.0	0.0	0.0	2.7	0.0	0.0
ASP	1	2	0	0	2	0	0	0	3	0	3	1	0	0	0	0	0	1	0	0
ASP	2.0	2.0	0.0	0.0	1.5	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
CYS	0	1	1	1	11	0	1	0	0	4	1	1	3	2	0	0	0	1	0	0
CYS	0.0	2.0	1.0	1.0	4.0	0.0	1.0	0.0	0.0	1.5	1.0	1.0	2.7	2.5	0.0	0.0	0.0	1.0	0.0	0.0
GLN	0	0	0	0	0	1	0	0	0	1	0	1	1	1	1	0	0	1	1	1
GLN	0.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	1.0	0.0	3.0	3.0	2.0	1.0	0.0	0.0	11.0	1.0	1.0
GLU	2	0	0	0	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	0
GLU	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	3.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	1	0	1	0	0	0	2	0	0	1	1	0	0	0	2	1
HIS	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	2.5	0.0	0.0	4.0	1.0	0.0	0.0	0.0	3.0	2.0
ILE	28	10	2	0	3	3	14	0	8	29	47	8	10	12	1	2	9	5	5	23
ILE	1.4	4.1	1.5	0.0	2.3	2.0	2.2	0.0	2.4	1.9	2.0	2.6	2.5	1.8	1.0	1.0	1.9	4.8	2.0	1.8
LEU	25	4	1	3	8	1	3	0	3	29	42	9	7	15	3	0	9	8	3	25
LEU	1.3	2.5	1.0	1.3	2.4	1.0	1.3	0.0	4.7	1.8	1.9	2.2	1.7	2.9	1.3	0.0	1.6	4.0	2.0	1.7
LYS	1	0	0	1	0	1	2	0	0	4	2	1	2	2	0	0	1	2	1	4
LYS	1.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	2.5	1.0	5.0	1.5	6.0	0.0	0.0	1.0	11.5	8.0	2.5
MET	6	4	2	0	1	0	2	0	1	5	6	0	1	1	0	0	3	4	1	3
MET	2.0	2.8	2.5	0.0	1.0	0.0	1.5	0.0	1.0	2.2	2.8	0.0	2.0	1.0	0.0	0.0	1.3	3.0	3.0	1.0
PHE	15	2	2	1	3	2	4	0	1	15	22	1	8	13	2	3	7	6	6	21
PHE	1.8	4.5	3.0	5.0	2.0	3.5	5.0	0.0	1.0	3.1	3.1	7.0	2.6	3.7	3.5	3.0	2.7	4.5	2.7	2.0
PRO	1	3	0	0	2	2	0	0	4	8	5	1	0	2	0	0	2	3	2	2
PRO	2.0	2.0	0.0	0.0	2.0	2.0	0.0	0.0	4.2	2.2	2.2	1.0	0.0	4.5	0.0	0.0	2.0	3.7	7.0	2.5
SER	4	0	0	1	0	1	1	0	3	1	0	1	0	4	1	0	2	1	0	5
SER	1.0	0.0	0.0	1.0	0.0	2.0	1.0	0.0	3.0	2.0	0.0	1.0	0.0	1.5	1.0	0.0	1.0	1.0	0.0	1.8
THR	9	1	0	0	4	3	0	0	2	1	6	1	1	2	0	1	4	1	2	1
THR	1.1	2.0	0.0	0.0	1.8	1.3	0.0	0.0	1.5	1.0	1.8	1.0	2.0	2.0	0.0	1.0	1.0	3.0	2.0	1.0
TRP	4	1	2	1	1	0	1	0	2	7	5	4	1	2	0	0	1	2	2	3
TRP	3.8	12.0	2.0	1.0	1.0	0.0	9.0	0.0	2.5	4.6	4.4	2.0	8.0	5.5	0.0	0.0	1.0	4.5	4.5	1.3
TYR	18	0	0	1	6	2	2	0	4	9	9	0	3	5	0	3	1	2	2	11
TYR	1.9	0.0	0.0	3.0	1.8	2.5	2.0	0.0	5.2	3.8	3.8	0.0	3.7	4.2	0.0	1.3	1.0	1.0	8.0	3.1
VAL	42	4	1	3	4	6	4	0	4	12	38	8	8	16	1	10	9	6	2	41
VAL	1.2	1.5	1.0	1.3	1.0	1.2	1.8	0.0	1.5	2.3	1.6	2.5	2.6	2.5	2.0	1.3	2.1	2.5	2.0	1.9

Table 70: Number of residue-residue interactions and average atom contacts for interactions between hydrophobic side-chain atoms. Interactions are between pairs of β -sheets.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	6	1	0	3	2	7	3	0	3	42	36	5	6	20	8	7	12	12	24	45
ALA	1.0	1.0	0.0	1.0	1.0	1.1	1.3	0.0	1.7	1.2	1.4	1.2	1.5	2.0	1.8	1.0	1.2	1.7	2.0	1.2
ARG	1	0	0	3	0	3	5	0	0	9	10	2	2	7	2	2	5	4	13	8
ARG	1.0	0.0	0.0	1.7	0.0	1.7	1.8	0.0	0.0	2.8	2.2	1.5	2.5	3.0	3.5	2.0	1.8	5.5	2.8	2.6
ASN	0	0	0	2	0	2	5	0	0	9	10	2	1	0	0	0	4	1	6	10
ASN	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	1.6	1.6	3.0	3.0	0.0	0.0	0.0	1.0	1.0	2.7	1.3
ASP	3	3	2	0	3	3	6	0	1	14	9	4	0	5	0	2	3	3	9	4
ASP	1.0	1.7	1.0	0.0	1.3	1.3	1.7	0.0	1.0	1.5	1.3	2.0	0.0	2.4	0.0	1.0	1.3	2.3	1.9	1.2
CYS	2	0	0	3	12	3	1	0	4	4	16	4	7	10	1	4	3	3	5	10
CYS	1.0	0.0	0.0	1.3	4.0	2.3	2.0	0.0	2.2	1.0	1.7	3.5	3.3	2.5	1.0	1.0	1.7	3.0	2.2	1.5
GLN	7	3	2	3	3	0	3	0	5	7	11	3	0	4	4	0	5	4	6	16
GLN	1.1	1.7	1.0	1.3	2.3	0.0	1.3	0.0	2.2	1.4	2.0	1.7	0.0	3.0	1.2	0.0	1.0	3.2	3.2	1.8
GLU	3	5	5	6	1	3	0	0	0	9	10	12	0	2	4	4	9	2	11	9
GLU	1.3	1.8	1.0	1.7	2.0	1.3	0.0	0.0	0.0	1.7	1.7	2.7	0.0	1.5	1.5	1.2	1.8	3.5	2.4	2.9
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	3	0	0	1	4	5	0	0	12	4	7	2	4	5	0	2	2	4	5	8
HIS	1.7	0.0	0.0	1.0	2.2	2.2	0.0	0.0	1.2	1.2	2.1	1.5	3.2	1.8	0.0	1.0	3.5	5.0	2.0	1.8
ILE	42	9	9	14	4	7	9	0	4	68	90	11	10	40	11	10	18	16	28	88
ILE	1.2	2.8	1.6	1.5	1.0	1.4	1.7	0.0	1.2	2.1	1.9	2.5	2.1	2.9	2.1	1.1	1.9	2.4	2.1	1.7
LEU	36	10	10	9	16	11	10	0	7	90	158	9	24	79	13	4	31	20	25	137
LEU	1.4	2.2	1.8	1.3	1.7	2.0	1.7	0.0	2.1	1.9	1.8	2.6	2.2	2.4	1.5	1.2	1.8	3.2	3.3	1.9
LYS	5	2	2	4	4	3	12	0	2	11	9	2	6	9	2	8	16	8	8	11
LYS	1.2	1.5	3.0	2.0	3.5	1.7	2.7	0.0	1.5	2.5	2.6	1.0	1.5	3.6	3.0	1.8	1.8	7.8	4.5	1.6
MET	6	2	1	0	7	0	0	0	4	10	24	6	6	17	6	4	2	4	4	21
MET	1.5	2.5	3.0	0.0	3.3	0.0	0.0	0.0	3.2	2.1	2.2	1.5	1.0	4.3	2.2	1.8	2.0	4.2	5.0	2.0
PHE	20	7	0	5	10	4	2	0	5	40	79	9	17	50	2	9	15	12	20	62
PHE	2.0	3.0	0.0	2.4	2.5	3.0	1.5	0.0	1.8	2.9	2.4	3.6	4.3	3.5	6.0	3.1	2.2	4.1	3.2	2.7
PRO	8	2	0	0	1	4	4	0	0	11	13	2	6	2	0	3	5	7	2	16
PRO	1.8	3.5	0.0	0.0	1.0	1.2	1.5	0.0	0.0	2.1	1.5	3.0	2.2	6.0	0.0	1.7	1.0	3.9	3.5	1.7
SER	7	2	0	2	4	0	4	0	2	10	4	8	4	9	3	10	12	1	7	13
SER	1.0	2.0	0.0	1.0	1.0	0.0	1.2	0.0	1.0	1.1	1.2	1.8	1.8	3.1	1.7	1.0	1.1	2.0	2.3	1.0
THR	12	5	4	3	3	5	9	0	2	18	31	16	2	15	5	12	12	3	17	22
THR	1.2	1.8	1.0	1.3	1.7	1.0	1.8	0.0	3.5	1.9	1.8	1.8	2.0	2.2	1.0	1.1	1.5	2.3	2.5	1.3
TRP	12	4	1	3	3	4	2	0	4	16	20	8	4	12	7	1	3	10	7	17
TRP	1.7	5.5	1.0	2.3	3.0	3.2	3.5	0.0	5.0	2.4	3.2	7.8	4.2	4.1	3.9	2.0	2.3	6.0	4.4	4.4
TYR	24	13	6	9	5	6	11	0	5	26	25	8	4	20	2	7	17	7	20	37
TYR	2.0	2.8	2.7	1.9	2.2	3.2	2.4	0.0	2.0	2.1	3.3	4.5	5.0	3.2	3.5	2.3	2.5	4.4	3.6	2.5
VAL	45	8	10	4	10	16	9	0	6	86	137	11	21	62	16	13	22	17	37	152
VAL	1.2	2.6	1.3	1.2	1.5	1.8	2.9	0.0	1.8	1.7	1.9	1.6	2.0	2.7	1.7	1.0	1.3	4.4	2.5	1.7

APPENDIX I

Table 71: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of α -helices with crossing angles between 0° and 30° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	2	0	0	0	0	0	0	0	1	8	7	0	2	0	0	1	0	0	2	4
ALA	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.9	1.4	0.0	2.0	0.0	0.0	1.0	0.0	0.0	1.5	1.0
ARG	0	0	1	0	0	0	0	0	1	1	1	0	0	0	0	0	1	1	0	1
ARG	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	5.0	4.0	0.0	0.0	0.0	0.0	0.0	2.0	8.0	0.0	6.0
ASN	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0
GLN	0	0	0	0	0	0	0	0	1	0	3	0	0	0	0	1	0	0	0	1
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	2.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0
GLU	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	1	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0
HIS	1.0	1.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.0	0.0
ILE	8	1	0	0	0	0	0	0	0	0	4	1	1	0	0	2	0	0	0	3
ILE	1.9	5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.8	3.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.3
LEU	7	1	0	0	2	3	1	0	0	4	14	0	3	7	0	1	0	1	5	2
LEU	1.4	4.0	0.0	0.0	2.5	2.0	2.0	0.0	0.0	1.8	2.1	0.0	1.3	3.0	0.0	1.0	0.0	8.0	3.8	2.5
LYS	0	0	0	1	0	0	1	0	0	1	0	0	0	0	0	1	0	0	0	1
LYS	0.0	0.0	0.0	1.0	0.0	0.0	4.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	2.0
MET	2	0	0	0	0	0	0	0	0	1	3	0	0	1	0	0	0	0	0	2
MET	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.3	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	1.0
PHE	0	0	0	0	0	0	0	0	0	0	7	0	1	12	0	0	0	2	0	1
PHE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	2.0	3.3	0.0	0.0	0.0	2.0	0.0	2.0
PRO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	1	0	0	0	0	1	0	0	0	2	1	1	0	0	0	0	0	0	3	0
SER	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0
THR	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
THR	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0
TRP	0	1	0	0	0	0	0	0	0	0	1	0	0	2	0	0	0	0	0	0
TRP	0.0	8.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	2	0	0	0	1	0	0	0	1	0	5	0	0	0	0	3	1	0	0	2
TYR	1.5	0.0	0.0	0.0	2.0	0.0	0.0	0.0	6.0	0.0	3.8	0.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	4.5
VAL	4	1	0	0	0	1	0	0	0	3	2	1	2	1	0	0	0	0	2	2
VAL	1.0	6.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.3	2.5	2.0	1.0	2.0	0.0	0.0	0.0	4.5	1.0	1.0

Table 72: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of α -helices with crossing angles between 30° and 60°.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	3	0	0	1	0	0	0	0	2	2	3	0	1	1	0	0	0	1	0	5
ALA	1.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	1.0	2.0	0.0	0.0	0.0	1.0	0.0	1.0
ARG	0	0	0	0	0	0	0	0	0	1	0	0	0	0	2	0	0	0	0	1
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	2.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	2
ASP	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
CYS	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	2.0
GLU	0	0	0	0	0	0	0	0	0	0	0	1	1	0	2	1	0	0	0	1
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	1.5	1.0	0.0	0.0	0.0	0.0	1.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	1	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	5
HIS	0.0	1.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0
ILE	2	1	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	2	3	1
ILE	1.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	2.0	1.0
LEU	5	0	0	1	1	0	0	0	0	3	2	0	1	3	4	0	0	0	2	5
LEU	1.0	0.0	0.0	2.0	1.0	0.0	0.0	0.0	0.0	2.0	1.0	0.0	1.0	1.7	1.2	0.0	0.0	0.0	2.0	1.4
LYS	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	1	0	4
LYS	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	5.0	0.0	2.2
MET	1	0	0	0	1	0	1	0	1	0	1	1	0	1	1	1	0	1	0	1
MET	1.0	0.0	0.0	0.0	2.0	0.0	1.0	0.0	4.0	0.0	1.0	1.0	0.0	2.0	1.0	1.0	0.0	3.0	0.0	2.0
PHE	1	0	0	0	0	0	0	0	0	0	3	0	1	6	1	0	0	0	0	2
PHE	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.7	0.0	2.0	2.0	4.0	0.0	0.0	0.0	0.0	1.5
PRO	0	2	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	1	0	2
PRO	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	4.0	0.0	0.0	0.0	3.0	0.0	1.0
SER	0	0	0	0	0	3	1	0	0	0	0	0	1	0	0	0	0	0	0	1
SER	0.0	0.0	0.0	0.0	0.0	1.3	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0
THR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	1	0	0	0	0	0	0	0	0	2	0	1	1	0	1	0	0	0	0	0
TRP	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	0.0	5.0	3.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	0	0	0	0	0	0	3	2	0	0	0	0	0	0	0	2	1
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.0
VAL	3	1	0	0	2	1	1	0	1	1	5	4	1	2	0	1	0	0	1	4
VAL	1.0	2.0	0.0	0.0	1.0	2.0	1.0	0.0	1.0	1.0	1.4	2.2	2.0	1.5	0.0	2.0	0.0	0.0	2.0	1.5

Table 73: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of α -helices with crossing angles between 60° and 90°.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	0	0	0	3	2	1	0	0	0	0	0	0	1	1
ALA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3	1.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	6.0	1.0
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	0	0	0	0	0	2	0	0	0	0	1	0	0	0	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	0	0	0	0	0	0	0	0	0	1	3	1	0	0	0	0	2	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	1.3	2.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	3	0	0	2	0	0	1	0	0	0	1	0	1	0	0	0	1	0	0	0
ILE	1.3	0.0	0.0	1.0	0.0	0.0	3.0	0.0	0.0	0.0	3.0	0.0	2.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
LEU	2	0	0	0	0	0	3	0	0	1	6	0	0	3	0	0	2	1	0	6
LEU	1.0	0.0	0.0	0.0	0.0	0.0	1.3	0.0	0.0	3.0	1.3	0.0	0.0	5.3	0.0	0.0	2.5	2.0	0.0	1.2
LYS	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
LYS	2.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2	0	0
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0
PHE	0	0	0	0	0	0	0	0	0	3	0	0	0	4	0	0	0	1	0	1
PHE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.3	0.0	0.0	0.0	4.0	0.0	0.0	0.0	1.0	0.0	1.0
PRO	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
PRO	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0
SER	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
THR	0	0	0	0	0	0	2	0	0	1	2	0	0	0	0	0	0	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	1.0	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	0	0	0	0	0	0	1	0	2	1	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	4.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TYR	6.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	1	0	0	0	0	0	0	0	0	0	6	0	0	1	1	1	0	0	0	2
VAL	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.2	0.0	0.0	1.0	2.0	1.0	0.0	0.0	0.0	0.0	2.0

Table 74: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of α -helices with crossing angles between 90° and 120° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	10	0	0	0	0	0	0	0	0	6	6	1	4	5	0	0	1	1	2	9
ALA	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.2	1.2	1.0	1.0	1.8	0.0	0.0	2.0	1.0	1.5	1.0
ARG	0	0	1	1	0	2	1	0	0	2	4	0	1	0	0	2	0	0	4	0
ARG	0.0	0.0	1.0	2.0	0.0	1.0	5.0	0.0	0.0	1.0	2.2	0.0	2.0	0.0	0.0	2.5	0.0	0.0	3.5	0.0
ASN	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1
ASN	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0
ASP	0	1	0	0	0	0	0	0	0	0	0	2	1	2	0	0	0	0	2	0
ASP	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	1.0	2.0	0.0	0.0	0.0	0.0	2.0	0.0
CYS	0	0	0	0	0	0	0	0	0	3	2	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	2	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	1	1	0
GLN	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	3.0	0.0
GLU	0	1	0	0	0	1	0	0	0	0	1	0	0	0	0	1	0	1	1	1
GLU	0.0	5.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	1.0	0.0	2.0	1.0	1.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	4	0	0	1	0	0	1	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	0.0	0.0	3.0	0.0	0.0	1.0	0.0	0.0	0.0
ILE	6	2	0	0	3	1	0	0	0	6	8	5	1	6	1	1	0	0	1	4
ILE	1.2	1.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	3.0	2.0	2.0	3.0	2.3	5.0	1.0	0.0	0.0	2.0	2.0
LEU	6	4	0	0	2	0	1	0	4	8	30	1	4	5	0	4	0	3	3	27
LEU	1.2	2.2	0.0	0.0	1.5	0.0	2.0	0.0	2.5	2.0	1.7	1.0	2.0	2.4	0.0	1.2	0.0	3.3	3.0	1.5
LYS	1	0	0	2	0	0	0	0	0	5	1	0	1	2	1	0	0	0	2	1
LYS	1.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	0.0	4.0	4.0	4.0	0.0	0.0	0.0	6.5	1.0
MET	4	1	0	1	0	0	0	0	0	1	4	1	0	4	0	0	1	0	0	2
MET	1.0	2.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	3.0	2.0	4.0	0.0	2.8	0.0	0.0	2.0	0.0	0.0	1.5
PHE	5	0	1	2	0	0	0	0	1	6	5	2	4	18	0	0	1	1	2	13
PHE	1.8	0.0	1.0	2.0	0.0	0.0	0.0	0.0	3.0	2.3	2.4	4.0	2.8	3.4	0.0	0.0	4.0	6.0	1.5	2.4
PRO	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	1	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.0	0.0	4.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0
SER	0	2	0	0	0	0	1	0	0	1	4	0	0	0	0	0	0	0	0	0
SER	0.0	2.5	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	1	0	0	0	0	0	0	0	1	0	0	0	1	1	2	0	0	0	0	1
THR	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	2.0	4.0	3.0	0.0	0.0	0.0	0.0	1.0
TRP	1	0	0	0	0	1	1	0	0	0	3	0	0	1	2	0	0	0	0	2
TRP	1.0	0.0	0.0	0.0	0.0	1.0	2.0	0.0	0.0	0.0	3.3	0.0	0.0	6.0	2.5	0.0	0.0	0.0	0.0	1.5
TYR	2	4	0	3	0	1	1	0	0	1	3	2	0	2	0	0	0	0	2	5
TYR	1.5	3.5	0.0	2.3	0.0	3.0	1.0	0.0	0.0	2.0	3.0	6.5	0.0	1.5	0.0	0.0	0.0	0.0	5.0	2.6
VAL	9	0	1	0	0	0	1	0	0	4	27	1	2	13	0	0	1	2	5	14
VAL	1.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0	1.5	1.0	1.5	2.4	0.0	0.0	1.0	1.5	2.6	2.0

Table 75: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of α -helices with crossing angles between 120° and 150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	4	2	1	1	0	2	2	0	0	4	19	2	0	3	0	1	2	0	1	9
ALA	1.0	1.5	2.0	1.0	0.0	1.5	1.0	0.0	0.0	1.2	1.2	1.5	0.0	1.7	0.0	1.0	1.0	0.0	1.0	1.3
ARG	2	0	0	0	2	0	0	0	0	0	5	0	0	0	0	0	0	1	1	7
ARG	1.5	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	1.8	0.0	0.0	0.0	0.0	0.0	0.0	11.0	3.0	1.3
ASN	1	0	0	0	0	0	0	0	1	2	0	1	0	0	0	0	1	0	0	0
ASN	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	1.0	0.0	6.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
ASP	1	0	0	0	0	0	1	0	0	0	4	0	0	1	0	0	0	0	1	0
ASP	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	2.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	2.0	0.0
CYS	0	2	0	0	0	0	0	0	0	1	1	0	2	0	0	0	0	0	0	1
CYS	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	1.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0
GLN	2	0	0	0	0	0	0	0	2	2	1	0	0	0	0	0	0	0	0	3
GLN	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3
GLU	2	0	0	3	0	0	0	0	3	2	3	6	3	2	0	0	2	1	0	6
GLU	1.0	0.0	0.0	1.3	0.0	0.0	0.0	0.0	1.0	2.0	2.7	1.5	1.7	6.0	0.0	0.0	3.0	1.0	0.0	3.2
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	1	0	0	0	3	0	0	0	1	0	0	4	0	2	0	0	3	1
HIS	0.0	0.0	4.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	1.8	0.0	2.5	0.0	0.0	8.7	2.0
ILE	4	0	2	0	1	2	2	0	0	4	12	3	0	5	1	0	1	2	3	7
ILE	1.2	0.0	1.0	0.0	3.0	2.0	2.0	0.0	0.0	3.5	1.4	2.3	0.0	1.8	1.0	0.0	1.0	5.0	2.3	2.1
LEU	19	5	0	4	1	1	3	0	1	12	56	1	3	7	4	5	1	4	8	13
LEU	1.2	1.8	0.0	2.0	1.0	1.0	2.7	0.0	1.0	1.4	1.6	1.0	2.0	2.3	1.2	1.8	2.0	5.0	3.2	1.2
LYS	2	0	1	0	0	0	6	0	0	3	1	0	0	0	0	0	0	2	2	3
LYS	1.5	0.0	6.0	0.0	0.0	0.0	1.5	0.0	0.0	2.3	1.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	5.5	2.0
MET	0	0	0	0	2	0	3	0	0	0	3	0	0	0	2	0	0	0	1	2
MET	0.0	0.0	0.0	0.0	2.0	0.0	1.7	0.0	0.0	0.0	2.0	0.0	0.0	0.0	4.5	0.0	0.0	0.0	4.0	4.0
PHE	3	0	0	1	0	0	2	0	4	5	7	0	0	8	1	2	2	1	0	5
PHE	1.7	0.0	0.0	1.0	0.0	0.0	6.0	0.0	1.8	1.8	2.3	0.0	0.0	4.5	1.0	1.0	2.5	5.0	0.0	3.8
PRO	2	0	0	0	0	0	0	0	0	1	4	0	0	1	0	0	1	1	2	1
PRO	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.2	0.0	0.0	1.0	0.0	0.0	1.0	4.0	2.0	3.0
SER	1	0	0	0	0	0	0	0	2	0	5	0	0	2	0	0	0	0	0	1
SER	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	0.0	1.8	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	2.0
THR	2	0	1	0	0	0	2	0	0	1	1	0	0	2	1	0	0	0	3	0
THR	1.0	0.0	1.0	0.0	0.0	0.0	3.0	0.0	0.0	1.0	2.0	0.0	0.0	2.5	1.0	0.0	0.0	0.0	1.7	0.0
TRP	0	1	0	0	0	0	1	0	0	2	4	2	0	1	1	0	0	0	2	2
TRP	0.0	11.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	5.0	5.0	3.0	0.0	5.0	4.0	0.0	0.0	0.0	3.5	2.0
TYR	1	1	0	1	0	0	0	0	3	3	8	2	1	0	2	0	3	2	2	1
TYR	1.0	3.0	0.0	2.0	0.0	0.0	0.0	0.0	8.7	2.3	3.2	5.5	4.0	0.0	2.0	0.0	1.7	3.5	4.0	1.0
VAL	9	7	0	0	1	1	4	0	1	7	13	3	2	5	1	1	0	2	1	16
VAL	1.3	1.3	0.0	0.0	2.0	2.0	3.0	0.0	2.0	2.1	1.2	2.0	4.0	3.8	3.0	2.0	0.0	2.0	1.0	2.1

Table 76: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of α -helices with crossing angles between 150° and 180° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	8	3	0	0	0	0	0	0	2	3	8	2	2	7	2	1	2	0	0	7
ALA	1.0	1.7	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	1.3	1.5	1.0	1.6	2.0	1.0	1.5	0.0	0.0	1.1
ARG	3	2	0	1	0	0	0	0	0	1	0	0	0	1	0	1	0	0	0	1
ARG	1.7	8.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	7.0	0.0	3.0	0.0	0.0	0.0	2.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
ASP	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0
CYS	0	0	0	0	4	0	0	0	0	1	1	0	0	3	0	0	0	0	1	0
CYS	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	2.0	3.0	0.0	0.0	2.3	0.0	0.0	0.0	0.0	2.0	0.0
GLN	0	0	0	0	0	0	0	0	1	1	1	0	2	2	0	0	0	0	0	2
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	1.0	0.0	2.0	3.0	0.0	0.0	0.0	0.0	0.0	1.0
GLU	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	1	0	1	2
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	2.0	0.0	1.0	0.0	8.0	1.5
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	2	0	0	0	0	1	0	0	0	0	0	0	0	1	0	2	0	0	0	2
HIS	2.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	1.0	0.0	0.0	0.0	2.0
ILE	3	1	0	0	1	1	0	0	0	0	4	0	1	2	0	0	2	0	0	1
ILE	1.0	2.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	0.0	3.2	0.0	1.0	3.0	0.0	0.0	1.5	0.0	0.0	2.0
LEU	8	0	0	0	1	1	1	0	0	4	8	0	0	14	2	0	1	0	3	4
LEU	1.3	0.0	0.0	0.0	3.0	1.0	2.0	0.0	0.0	3.2	1.7	0.0	0.0	2.8	2.0	0.0	2.0	0.0	1.7	2.0
LYS	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
LYS	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5
MET	2	0	0	0	0	2	0	0	0	1	0	0	0	2	0	0	0	0	0	2
MET	1.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	3.5
PHE	7	1	0	0	3	2	0	0	1	2	14	0	2	0	0	0	0	0	1	2
PHE	1.6	7.0	0.0	0.0	2.3	3.0	0.0	0.0	2.0	3.0	2.8	0.0	4.0	0.0	0.0	0.0	0.0	0.0	3.0	1.0
PRO	2	0	0	0	0	0	1	0	0	0	2	0	0	0	0	0	0	0	0	2
PRO	2.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0
SER	1	1	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	0	0	0
SER	1.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
THR	2	0	0	0	0	0	1	0	0	2	1	0	0	0	0	1	0	0	0	0
THR	1.5	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.5	2.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	1	1	0	1	0	0	0	3	0	0	1	0	0	0	0	0	0
TYR	0.0	0.0	0.0	2.0	2.0	0.0	8.0	0.0	0.0	0.0	1.7	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	7	1	0	0	0	2	2	0	2	1	4	2	2	2	2	0	0	0	0	14
VAL	1.1	2.0	0.0	0.0	0.0	1.0	1.5	0.0	2.0	2.0	2.0	2.5	3.5	1.0	3.0	0.0	0.0	0.0	0.0	1.3

Table 77: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of α -helices with crossing angles between -30° and 0° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	4	0	0	0	0	1	0	0	0	5	1	1	1	2	0	0	0	0	1	4
ALA	1.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	1.4	1.0	1.0	2.0	2.5	0.0	0.0	0.0	0.0	7.0	2.0
ARG	0	0	0	0	0	0	0	0	0	2	1	0	1	0	1	1	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	1.0	0.0	2.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	1	0	0	1	0	1	1	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
GLN	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	2
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	5	2	0	0	0	0	0	0	0	2	4	2	0	3	0	0	2	0	2	3
ILE	1.4	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	1.5	3.0	0.0	5.7	0.0	0.0	1.5	0.0	1.5	2.0
LEU	1	1	0	0	0	0	2	0	1	4	6	2	2	0	1	1	4	0	0	3
LEU	1.0	1.0	0.0	0.0	0.0	0.0	1.5	0.0	2.0	1.5	1.3	2.0	2.0	0.0	1.0	1.0	1.2	0.0	0.0	2.0
LYS	1	0	1	2	0	0	0	0	0	2	2	0	0	0	0	0	0	0	0	0
LYS	1.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	3.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	1	1	0	0	0	1	0	0	0	0	2	0	0	0	0	0	1	0	0	2
MET	2.0	2.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	1.0
PHE	2	0	1	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	2	0
PHE	2.5	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	5.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.0	0.0
PRO	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	1
PRO	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0
SER	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
SER	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	0	0	0	0	0	0	0	2	4	0	1	0	0	0	0	0	0	1
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	1.2	0.0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.0	0.0	0.0
TYR	1	0	0	0	0	0	0	0	0	2	0	0	0	2	1	0	0	0	0	0
TYR	7.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	6.0	1.0	0.0	0.0	0.0	0.0	0.0
VAL	4	0	0	0	0	0	2	0	0	3	3	0	2	0	1	0	1	0	0	0
VAL	2.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	2.0	2.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0

Table 78: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of α -helices with crossing angles between -60° and -30° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	9	2	2	1	0	1	2	0	0	6	11	3	5	6	0	3	3	3	1	9
ALA	1.0	1.0	1.0	1.0	0.0	1.0	2.0	0.0	0.0	1.7	1.4	1.0	1.4	1.8	0.0	1.0	1.0	1.7	6.0	1.1
ARG	2	2	0	0	1	0	1	0	1	3	1	0	1	1	2	1	0	0	0	0
ARG	1.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	1.0	2.3	1.0	0.0	2.0	1.0	4.0	2.0	0.0	0.0	0.0	0.0
ASN	2	0	0	1	0	1	0	0	2	0	1	0	1	0	0	0	0	0	0	0
ASN	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.5	0.0	1.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	1	0	1	2	0	0	1	0	0	0	0	1	1	3	0	0	0	0	0	0
ASP	1.0	0.0	1.0	2.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	2.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	1	0	0	0	0	1	0	0	2	3	0	3	1	1	0	0	0	0	2
CYS	0.0	1.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	2.0	1.0	0.0	1.0	2.0	1.0	0.0	0.0	0.0	0.0	1.0
GLN	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	1
GLN	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	2.0
GLU	2	1	0	1	1	0	0	0	1	2	2	1	0	4	0	1	0	0	0	0
GLU	2.0	4.0	0.0	1.0	2.0	0.0	0.0	0.0	2.0	1.5	2.0	3.0	0.0	4.2	0.0	1.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	2	0	0	0	0	0	1	0	0	2	1	0	3	1	0	3	3	1	0	0
HIS	1.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	1.5	6.0	0.0	1.0	8.0	0.0	1.3	3.0	1.0	0.0	0.0
ILE	6	3	0	0	2	0	2	0	2	4	8	1	1	4	0	3	0	3	2	8
ILE	1.7	2.3	0.0	0.0	2.0	0.0	1.5	0.0	1.5	3.0	2.2	1.0	1.0	3.5	0.0	1.3	0.0	3.3	6.5	2.2
LEU	9	1	1	0	2	0	2	0	1	8	16	2	8	5	2	1	4	4	3	11
LEU	1.4	1.0	1.0	0.0	1.0	0.0	2.0	0.0	6.0	2.2	2.2	1.5	1.8	3.0	1.5	1.0	2.0	3.2	2.7	1.9
LYS	3	0	0	1	0	0	1	0	0	1	2	0	0	0	0	1	0	0	2	2
LYS	1.0	0.0	0.0	1.0	0.0	0.0	3.0	0.0	0.0	1.0	1.5	0.0	0.0	0.0	0.0	1.0	0.0	0.0	3.0	2.0
MET	5	1	1	1	3	0	0	0	3	1	8	0	0	2	0	0	0	0	0	3
MET	1.4	2.0	3.0	2.0	1.0	0.0	0.0	0.0	1.0	1.0	1.8	0.0	0.0	2.5	0.0	0.0	0.0	0.0	0.0	1.3
PHE	6	1	0	3	1	0	4	0	1	4	5	0	2	2	0	1	0	1	2	3
PHE	1.8	1.0	0.0	4.0	2.0	0.0	4.2	0.0	8.0	3.5	3.0	0.0	2.5	5.0	0.0	1.0	0.0	6.0	3.0	3.3
PRO	0	2	0	0	1	0	2	0	0	0	6	0	0	0	0	0	3	1	0	6
PRO	0.0	2.0	0.0	0.0	1.0	0.0	1.5	0.0	0.0	0.0	1.3	0.0	0.0	0.0	0.0	0.0	4.0	2.0	0.0	2.2
SER	3	1	0	0	0	1	1	0	3	3	1	1	0	1	0	0	0	0	1	1
SER	1.0	2.0	0.0	0.0	0.0	1.0	1.0	0.0	1.3	1.3	1.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	2.0
THR	3	0	0	0	0	0	0	0	3	0	4	0	0	0	3	0	0	0	0	1
THR	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	2.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	1.0
TRP	3	0	0	0	0	0	0	0	1	3	4	0	0	1	1	0	0	0	0	0
TRP	1.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	3.3	3.2	0.0	0.0	6.0	2.0	0.0	0.0	0.0	0.0	0.0
TYR	1	0	0	0	0	0	0	0	0	2	3	2	0	2	0	1	0	0	0	2
TYR	6.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.5	2.7	3.0	0.0	3.0	0.0	1.0	0.0	0.0	0.0	3.5
VAL	11	0	0	2	0	1	0	0	4	8	11	2	3	3	8	1	1	0	2	4
VAL	1.1	0.0	0.0	1.0	0.0	2.0	0.0	0.0	2.2	2.2	1.9	2.0	1.3	3.3	1.9	2.0	1.0	0.0	3.5	1.5

Table 79: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of α -helices with crossing angles between -90° and -60° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	2	2	0	1	1	0	2	0	1	4	2	0	0	3	1	0	0	0	0	3
ALA	1.0	1.0	0.0	2.0	1.0	0.0	2.0	0.0	1.0	1.5	1.5	0.0	0.0	2.0	1.0	0.0	0.0	0.0	0.0	1.0
ARG	2	0	0	0	0	0	0	0	0	1	0	0	1	0	0	1	0	0	0	1
ARG	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0	0.0	0.0	1.0	0.0	0.0	0.0	2.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.0	0.0
ASP	1	0	0	0	0	0	0	0	2	1	0	0	0	1	0	0	1	0	0	0
ASP	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	3.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0
CYS	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
CYS	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	0	1	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0
GLU	2	0	0	0	0	0	0	0	0	1	1	2	1	0	0	1	0	2	0	0
GLU	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	1.0	2.0	0.0	0.0	3.0	0.0	2.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	1	0	0	2	0	0	0	0	0	0	2	0	0	2	0	0	0	0	0	0
HIS	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	3.5	0.0	0.0	0.0	0.0	0.0	0.0
ILE	4	1	0	1	0	0	1	0	0	6	9	1	0	2	0	0	1	2	0	4
ILE	1.5	1.0	0.0	3.0	0.0	0.0	2.0	0.0	0.0	1.3	1.6	3.0	0.0	6.5	0.0	0.0	1.0	5.0	0.0	2.0
LEU	2	0	0	0	1	5	1	0	2	9	36	1	2	5	1	1	1	3	3	11
LEU	1.5	0.0	0.0	0.0	3.0	2.0	2.0	0.0	2.0	1.6	1.6	1.0	1.0	2.4	2.0	1.0	1.0	1.7	2.0	1.2
LYS	0	0	0	0	0	0	2	0	0	1	1	0	0	0	1	0	0	0	0	0
LYS	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	3.0	1.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	0.0	0.0
MET	0	1	0	0	0	0	1	0	0	0	2	0	0	1	0	0	0	2	0	1
MET	0.0	2.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	1.0	0.0	0.0	4.0	0.0	0.0	0.0	1.5	0.0	1.0
PHE	3	0	0	1	0	0	0	0	2	2	5	0	1	6	1	0	0	0	0	2
PHE	2.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	3.5	6.5	2.4	0.0	4.0	1.0	2.0	0.0	0.0	0.0	0.0	3.0
PRO	1	0	0	0	0	0	0	0	0	0	1	1	0	1	0	0	0	0	0	0
PRO	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	5.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	1	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0
SER	0.0	1.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	0	1	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	2
THR	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0
TRP	0	0	0	0	0	1	2	0	0	2	3	0	2	0	0	0	0	0	4	1
TRP	0.0	0.0	0.0	0.0	0.0	2.0	2.0	0.0	0.0	5.0	1.7	0.0	1.5	0.0	0.0	0.0	0.0	0.0	1.5	3.0
TYR	0	0	1	0	0	0	0	0	0	0	3	0	0	0	0	0	0	4	0	3
TYR	0.0	0.0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	4.3
VAL	3	1	0	0	0	0	0	0	0	4	11	0	1	2	0	0	2	1	3	6
VAL	1.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.2	0.0	1.0	3.0	0.0	0.0	2.0	3.0	4.3	1.3

Table 80: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of α -helices with crossing angles between -120° and -90° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	4	0	0	1	0	0	1	0	0	0	2	0	0	1	0	3	0	1	0	2
ALA	1.0	0.0	0.0	2.0	0.0	0.0	1.0	0.0	0.0	0.0	1.5	0.0	0.0	2.0	0.0	1.0	0.0	1.0	0.0	1.0
ARG	0	0	0	0	0	0	0	0	0	0	4	0	0	1	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.8	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	1	2
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.5
ASP	1	0	0	0	1	0	0	0	0	2	0	1	0	0	0	2	0	0	1	0
ASP	2.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	3.0	0.0
CYS	0	0	0	1	2	0	0	0	2	0	2	0	0	2	0	1	0	0	0	0
CYS	0.0	0.0	0.0	2.0	4.0	0.0	0.0	0.0	2.0	0.0	1.0	0.0	0.0	2.0	0.0	1.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	1	0	0	0	0	0	0	0	0	1	3	2	0	0	0	0	0	0	2	2
GLU	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.7	1.5	0.0	0.0	0.0	0.0	0.0	0.0	5.5	2.5
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	2	0	0	0	0	0	1	0	0	1	0	1	0	0	0	0
HIS	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	5.0	0.0	1.0	0.0	0.0	0.0	0.0
ILE	0	0	0	2	0	0	1	0	0	0	4	0	0	0	0	0	0	1	1	0
ILE	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	2.8	0.0	0.0	0.0	0.0	0.0	0.0	1.0	5.0	0.0
LEU	2	4	0	0	2	2	3	0	1	4	14	1	0	7	0	0	9	1	4	7
LEU	1.5	1.8	0.0	0.0	1.0	2.0	1.7	0.0	1.0	2.8	1.7	1.0	0.0	3.3	0.0	0.0	2.0	2.0	3.0	1.1
LYS	0	0	0	1	0	0	2	0	0	0	1	0	0	2	0	0	0	0	0	0
LYS	0.0	0.0	0.0	1.0	0.0	0.0	1.5	0.0	0.0	0.0	1.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	1	0
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.0	0.0	1.0	0.0
PHE	1	1	0	0	2	0	0	0	1	0	7	2	0	0	0	1	0	1	2	3
PHE	2.0	2.0	0.0	0.0	2.0	0.0	0.0	0.0	5.0	0.0	3.3	2.0	0.0	0.0	0.0	3.0	0.0	5.0	4.5	4.7
PRO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	2	3	1	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.5	4.0	1.0	0.0
SER	3	0	3	2	1	0	0	0	1	0	0	0	0	1	1	0	0	0	1	3
SER	1.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	3.0	2.0	0.0	0.0	0.0	2.0	1.0
THR	0	0	0	0	0	0	0	0	0	0	9	0	2	0	1	0	0	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	5.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0
TRP	1	0	0	0	0	0	0	0	0	1	1	0	0	1	1	0	0	4	1	0
TRP	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.0	0.0	0.0	5.0	7.0	0.0	0.0	4.0	1.0	0.0
TYR	0	0	1	0	0	0	2	0	0	1	4	0	1	2	1	1	0	1	0	2
TYR	0.0	0.0	1.0	0.0	0.0	0.0	5.5	0.0	0.0	5.0	3.0	0.0	1.0	4.5	1.0	2.0	0.0	1.0	0.0	2.0
VAL	2	0	2	0	0	0	2	0	0	0	7	0	0	3	0	3	0	0	2	2
VAL	1.0	0.0	1.5	0.0	0.0	0.0	2.5	0.0	0.0	0.0	1.1	0.0	0.0	4.7	0.0	1.0	0.0	0.0	2.0	2.0

Table 81: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. - Interactions are between pairs of α -helices with crossing angle between -150° and -120° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	1	0	0	0	1	9	0	1	1	2	0	0	1	1	1
ALA	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	1.4	0.0	2.0	6.0	1.0	0.0	0.0	6.0	2.0	1.0
ARG	0	0	0	1	0	0	1	0	0	0	2	0	0	1	0	0	0	0	1	0
ARG	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	1.5	0.0	0.0	6.0	0.0	0.0	0.0	0.0	9.0	0.0
ASN	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	0	1	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	6.0	0.0	0.0	0.0	1.0	0.0	0.0
ASP	0	1	0	0	0	0	2	0	0	0	1	0	0	0	0	0	0	0	1	0
ASP	0.0	1.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0
CYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	1	0	0	0	0	0	0	0	0	1	0	0	1	1	0	0	0	0	0	0
GLN	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLU	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	2	0	0	0	0	1	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	1	0	1	0	0	1	0	0	0	0	6	0	0	2	0	0	0	1	2	1
ILE	1.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	1.5	0.0	0.0	0.0	4.0	2.0	1.0
LEU	9	2	1	1	0	0	0	0	1	6	10	2	2	4	0	0	1	7	2	3
LEU	1.4	1.5	1.0	1.0	0.0	0.0	0.0	0.0	2.0	1.5	1.2	2.0	1.5	2.5	0.0	0.0	1.0	3.9	4.0	1.0
LYS	0	0	0	0	0	0	0	0	0	0	2	0	1	0	0	0	0	0	0	2
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
MET	1	0	0	0	0	1	0	0	0	0	2	1	0	3	0	0	1	0	0	0
MET	2.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.5	1.0	0.0	2.7	0.0	0.0	3.0	0.0	0.0	0.0
PHE	1	1	1	0	0	1	0	0	0	2	4	0	3	4	0	0	0	3	1	3
PHE	6.0	6.0	6.0	0.0	0.0	4.0	0.0	0.0	0.0	1.5	2.5	0.0	2.7	3.5	0.0	0.0	0.0	4.7	1.0	1.3
PRO	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0
THR	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	1	0	1	0	0	0	0	0	0	1	7	0	0	3	0	1	0	0	0	4
TRP	6.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	3.9	0.0	0.0	4.7	0.0	2.0	0.0	0.0	0.0	3.5
TYR	1	1	0	1	0	0	0	0	0	2	2	0	0	1	0	0	0	0	0	0
TYR	2.0	9.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	2.0	4.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	1	0	0	0	0	2	2	0	0	1	3	2	0	3	0	0	0	4	0	4
VAL	1.0	0.0	0.0	0.0	0.0	1.0	3.5	0.0	0.0	1.0	1.0	1.0	0.0	1.3	0.0	0.0	0.0	3.5	0.0	1.5

Table 82: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of α -helices with crossing angles between -180° and -150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	0	0	0	4	2	0	0	1	0	0	1	0	0	2
ALA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.2	1.5	0.0	0.0	2.0	0.0	0.0	1.0	0.0	0.0	1.0
ARG	0	0	0	0	1	0	0	0	0	2	0	0	1	0	0	0	1	0	0	0
ARG	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	5.5	0.0	0.0	3.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
CYS	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	3	0	0	2
GLN	0.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3	0.0	0.0	1.5
GLU	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	13.0	0.0
ILE	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	1	1	0
ILE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	5.0	7.0	0.0
LEU	2	0	0	0	0	0	0	0	0	1	4	0	0	1	0	0	2	0	0	2
LEU	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.5	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	3.0
LYS	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	1	0	0
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
MET	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	3
MET	0.0	0.0	0.0	0.0	0.0	3.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.7
PHE	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	1	2
PHE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	0.0	3.0	0.0	0.0	0.0	0.0	1.0	3.5
PRO	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
THR	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
TRP	0	0	0	0	1	0	0	0	0	0	0	0	0	2	1	0	0	0	0	1
TRP	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	3.0	0.0	0.0	0.0	0.0	4.0
TYR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0
VAL	2	0	0	0	0	0	0	0	0	0	2	0	1	0	0	0	1	1	0	3
VAL	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	1.0	0.0	0.0	0.0	1.0	1.0	0.0	1.7

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	1	0	0	0	0	1	2	1	0	0	0	1	0	0	0	1
ALA	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	1.5	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	3.0
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLU	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ILE	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LEU	0	0	0	1	0	0	0	0	0	3	2	0	0	2	0	0	0	0	0	0
LEU	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0
LYS	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
MET	1.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHE	0	0	0	1	0	0	0	0	0	0	1	0	1	0	0	0	0	1	1	0
PHE	0.0	0.0	0.0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	11.0	2.0	0.0
PRO	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	0	0	0	0	0	2	0	2	0	0	0	0	0	2	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	2.0	0.0	0.0	0.0	0.0	0.0	4.5	0.0	0.0
TYR	2	0	0	0	0	1	0	0	0	0	1	0	1	0	0	0	0	0	0	0
TYR	2.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	5.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
VAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0

Table 84: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between α -helices and β -sheets with crossing angles between 30° and 60° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	1	0	0	0	0	1	0	0	1	0	0	0	0	1	1
ALA	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	1.0
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	0	2	0	0	0	0	0	0	0	1	4	0	1	1	0	0	1	0	0	0
ILE	0.0	5.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.8	0.0	6.0	2.0	0.0	0.0	2.0	0.0	0.0	0.0
LEU	0	0	0	0	1	0	0	0	0	1	1	0	0	1	0	0	1	1	0	1
LEU	0.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	0.0	1.0	2.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	2.0
LYS	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHE	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0
PHE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PRO	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	1	0	0	1	0	1	0	0	0	0	1	0	0	0	0	0	0	0	1	1
TYR	3.0	0.0	0.0	3.0	0.0	1.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	4.0
VAL	2	0	0	0	0	0	1	0	0	0	2	0	0	0	0	0	2	0	0	0
VAL	1.5	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0	2.5	0.0	0.0	0.0

Table 85: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between α -helices and β -sheets with crossing angles between 60° and 90° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	1	0	0	1
ALA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	0.0	0.0	2.0	0.0	0.0	2.0	0.0	0.0	1.0
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0
ASP	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASP	2.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
CYS	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	1	0	0	0	0	0	0	0	3	3	2	0	1	1	0	0	0	0	1	1
ILE	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.7	3.0	2.0	0.0	2.0	4.0	0.0	0.0	0.0	0.0	2.0	2.0
LEU	4	0	0	0	0	0	1	0	0	2	0	1	2	2	1	0	0	0	0	2
LEU	1.2	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	4.5	0.0	2.0	1.0	5.0	1.0	0.0	0.0	0.0	0.0	2.0
LYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	2
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.0	2.5
MET	2	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0
MET	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0
PHE	1	0	2	0	0	0	0	0	0	0	2	0	0	2	1	0	2	0	1	0
PHE	2.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	1.0	2.0	0.0	3.0	0.0	6.0	0.0
PRO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	1	0	0	0	0	0	1	0	1	1	0	0	0	1	0	0	0	0	0	0
SER	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	3.0	2.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	1	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0
TRP	1	0	0	0	0	0	0	0	1	1	0	1	0	0	0	0	0	0	0	0
TRP	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	8.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	2	0	0	0	0
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0
VAL	0	0	0	0	0	0	0	0	1	0	2	0	1	2	0	2	0	0	0	1
VAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.5	0.0	6.0	2.5	0.0	2.0	0.0	0.0	0.0	3.0

Table 86: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between α -helices and β -sheets with crossing angles between 90° and 120° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	2	0	0	0	0	1	0	0	2	1	1	0	0	1	0	0	0	0	0	2
ALA	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	1.0
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
CYS	0	0	0	0	3	0	0	0	0	3	1	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	11.0	0.0	1.0
GLU	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
ILE	0	0	1	0	0	1	1	0	1	0	5	0	0	2	1	0	0	0	0	3
ILE	0.0	0.0	1.0	0.0	0.0	3.0	1.0	0.0	2.0	0.0	3.2	0.0	0.0	1.5	1.0	0.0	0.0	0.0	0.0	1.7
LEU	4	1	0	0	0	1	2	0	2	2	7	0	1	1	1	0	0	0	1	1
LEU	1.2	3.0	0.0	0.0	0.0	1.0	1.0	0.0	4.0	1.0	2.4	0.0	1.0	1.0	1.0	0.0	0.0	0.0	1.0	3.0
LYS	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	8.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHE	0	0	0	0	0	1	0	0	0	2	1	0	3	2	0	0	0	0	1	1
PHE	0.0	0.0	0.0	0.0	0.0	6.0	0.0	0.0	0.0	1.5	3.0	0.0	3.0	5.5	0.0	0.0	0.0	0.0	1.0	3.0
PRO	0	2	0	0	1	1	0	0	3	1	0	0	0	0	0	0	0	0	0	1
PRO	0.0	2.5	0.0	0.0	2.0	1.0	0.0	0.0	5.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
SER	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0
THR	2	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0
THR	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
TRP	1	0	0	0	0	0	0	0	0	1	2	0	0	0	0	0	0	0	0	0
TRP	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.0	4.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	1	0	0	0	1	0	1	0	0	1	0	0	0	1	0	0	0	0	0	0
TYR	1.0	0.0	0.0	0.0	2.0	0.0	3.0	0.0	0.0	1.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	1	1	0	1	1	1	0	0	1	1	2	0	3	0	1	0	0	0	0	4
VAL	1.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	1.0	1.0	1.0	3.0	0.0	1.3	0.0	1.0	0.0	0.0	0.0	1.5

Table 87: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between α -helices and β -sheets with crossing angles between 120° and 150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	6	0	0	0	0	0	0	0	0	3	1	0	1	0	0	1	3	2	0	1
ALA	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.0	0.0	1.0	0.0	0.0	1.0	1.0	3.5	0.0	1.0
ARG	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASP	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	0	0	2	0	1	0	0	0	0	0	0	2	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	4.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	3.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	7	2	0	0	1	0	3	0	0	5	9	2	0	1	0	1	1	1	0	3
ILE	1.4	4.0	0.0	0.0	2.0	0.0	2.0	0.0	0.0	1.2	1.8	2.5	0.0	2.0	0.0	1.0	2.0	10.0	0.0	1.3
LEU	2	0	1	0	4	0	0	0	0	6	7	5	0	1	0	0	1	1	0	5
LEU	1.0	0.0	1.0	0.0	1.5	0.0	0.0	0.0	0.0	1.7	1.7	2.2	0.0	3.0	0.0	0.0	3.0	3.0	0.0	1.6
LYS	1	0	0	0	0	0	1	0	0	1	1	0	1	0	0	0	0	0	0	0
LYS	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	2	1	2	0	0	0	0	0	0	0	1	0	1	0	0	0	1	3	0	0
MET	3.0	3.0	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	2.0	0.0	0.0	0.0	1.0	1.7	0.0	0.0
PHE	4	1	0	0	0	0	1	0	0	5	5	0	1	2	0	1	1	1	1	9
PHE	1.8	6.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	1.8	4.2	0.0	2.0	3.5	0.0	4.0	1.0	2.0	5.0	1.9
PRO	0	1	0	0	0	1	0	0	0	1	0	1	0	0	0	0	0	1	0	0
PRO	0.0	1.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	3.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	2
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	2.0
THR	2	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0
THR	1.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
TRP	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	1
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	8.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0
TYR	4	0	0	0	1	0	1	0	1	3	2	0	2	3	0	0	1	1	0	1
TYR	2.5	0.0	0.0	0.0	1.0	0.0	1.0	0.0	1.0	6.3	6.0	0.0	4.0	5.3	0.0	0.0	1.0	1.0	0.0	1.0
VAL	9	1	0	2	0	1	2	0	0	3	8	1	2	1	0	1	4	2	0	9
VAL	1.1	2.0	0.0	1.5	0.0	1.0	2.5	0.0	0.0	2.3	1.9	2.0	3.0	4.0	0.0	1.0	1.8	3.5	0.0	2.3

Table 88: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between α -helices and β -sheets with crossing angles between 150° and 180° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	2	0	0	0	0	0	0	0	0	4	0	0	1	2	0	1	3	1	0	2
ALA	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.2	0.0	0.0	2.0	2.0	0.0	1.0	1.0	2.0	0.0	1.5
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	0	0	0	0	3	0	2	0	0	0	0	0	0	0	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	1	0	1	0	0	0	0	1	0	1	0	1	0	0	0	0	0	0
CYS	0.0	0.0	1.0	0.0	4.0	0.0	0.0	0.0	0.0	3.0	0.0	1.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLU	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	5.0	0.0
ILE	8	3	0	0	0	2	2	0	3	14	7	1	3	1	0	1	3	1	1	5
ILE	1.4	3.3	0.0	0.0	0.0	1.5	3.0	0.0	2.0	2.0	2.1	3.0	1.3	1.0	0.0	1.0	2.0	3.0	1.0	1.4
LEU	7	2	0	0	0	0	0	0	0	7	5	0	3	1	0	0	2	1	1	8
LEU	1.3	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.4	2.2	0.0	1.7	7.0	0.0	0.0	1.5	14.0	1.0	1.5
LYS	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	1	1	0	2
LYS	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	12.0	0.0	2.5
MET	1	0	0	0	0	0	1	0	0	3	1	0	0	0	0	0	1	0	0	1
MET	3.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	2.3	5.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	1.0
PHE	4	1	0	0	0	1	0	0	1	6	3	0	1	1	0	1	3	2	1	3
PHE	1.8	3.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	4.7	3.3	0.0	2.0	1.0	0.0	1.0	3.0	3.0	1.0	2.3
PRO	0	0	0	0	0	0	0	0	0	1	2	0	0	0	0	0	1	0	1	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	2.0	0.0
SER	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0
SER	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
THR	4	0	0	0	0	0	0	0	2	0	0	1	0	0	0	0	0	0	0	0
THR	1.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	0	0	2	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	1	0	0	0	0	0	0	0	1	0	2	0	0	0	0	0	0	1	0	4
TYR	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	3.8
VAL	22	0	0	0	1	1	0	0	2	4	11	4	2	5	1	3	0	1	0	14
VAL	1.1	0.0	0.0	0.0	1.0	1.0	0.0	0.0	2.0	3.5	1.5	2.5	2.0	2.4	2.0	1.3	0.0	2.0	0.0	1.9

[illegible]

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	1.	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
ALA	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARG	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	0	1	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0
ASP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	1	0	0	0	0	0	0	0	0	2	3	0	0	0	0	0	0	2	0	4
ILE	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	2.3	0.0	0.0	0.0	0.0	0.0	0.0	4.5	0.0	1.5
LEU	3	0	0	1	0	0	0	0	0	2	3	0	0	0	0	0	2	3	0	3
LEU	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.5	1.7	0.0	0.0	0.0	0.0	0.0	2.0	3.7	0.0	1.7
LYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHE	1	0	0	0	2	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0
PHE	1.0	0.0	0.0	0.0	2.5	0.0	0.0	0.0	0.0	0.0	1.0	7.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PRO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	1.0	0.0	9.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
TYR	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.5
VAL	1	1	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	1
VAL	1.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0

Table 90: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between α -helices and β -sheets with crossing angles between -60° and -30° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	1	0	2
ALA	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	1.0
ARG	0	0	1	0	0	0	0	0	0	1	1	0	0	1	0	0	0	0	0	0
ARG	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASP	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0
ILE	0	1	1	0	1	0	2	0	0	3	7	1	0	1	0	0	2	0	1	2
ILE	0.0	1.0	2.0	0.0	3.0	0.0	2.5	0.0	0.0	1.7	2.0	1.0	0.0	1.0	0.0	0.0	2.0	0.0	2.0	2.0
LEU	0	0	0	0	3	0	0	0	0	1	1	1	0	3	0	0	0	0	0	0
LEU	0.0	0.0	0.0	0.0	2.7	0.0	0.0	0.0	0.0	2.0	1.0	1.0	0.0	1.3	0.0	0.0	0.0	0.0	0.0	0.0
LYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
PHE	1	0	0	0	1	0	1	0	0	0	1	0	0	2	0	1	0	0	1	6
PHE	3.0	0.0	0.0	0.0	1.0	0.0	13.0	0.0	0.0	2.0	0.0	0.0	0.0	6.5	0.0	4.0	0.0	0.0	1.0	1.2
PRO	0	0	0	0	0	0	0	0	0	3	1	0	0	1	0	0	1	0	0	1
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.7	2.0	0.0	0.0	4.0	0.0	0.0	2.0	0.0	0.0	4.0
SER	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	2
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	1.5
THR	0	0	0	0	0	0	0	0	0	0	1	0	0	2	0	0	0	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	1	0	0	0	0	0	0	0	1	0	0	0	0	2	0	0	0	0	1	0
TRP	6.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	5.5	0.0	0.0	0.0	0.0	8.0	0.0
TYR	5	0	0	0	4	0	0	0	0	2	1	0	0	0	0	0	0	0	1	3
TYR	1.8	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	2.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	15.0	2.3
VAL	2	1	1	0	1	0	0	0	0	0	4	1	0	0	0	0	0	0	0	3
VAL	2.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.5	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0

Table 91: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between α -helices and β -sheets with crossing angles between -90° and -60° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0
ALA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
ASP	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	1	0	0	0	0	0	2	0	1	1	4	0	2	2	0	0	0	0	0	3
ILE	1.0	0.0	0.0	0.0	0.0	0.0	3.5	0.0	6.0	1.0	1.2	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	2.0
LEU	0	0	0	1	0	0	0	0	1	3	4	0	0	1	1	0	0	0	0	1
LEU	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	6.0	1.3	1.2	0.0	0.0	1.0	2.0	0.0	0.0	0.0	0.0	2.0
LYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0
PHE	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
PHE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0
PRO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0
THR	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	1	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0
TYR	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	1
VAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	2.0

Table 92: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between α -helices and β -sheets with crossing angles between -120° and -90° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
ALA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	0	0	0	0	0	0	0	0	0	0	2	0	1	1	0	0	1	1	0	1
ILE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	5.0	1.0	0.0	0.0	2.0	2.0	0.0	1.0
LEU	1	1	0	0	0	0	0	0	0	1	4	1	1	2	0	0	1	0	0	2
LEU	1.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	2.2	3.0	4.0	3.5	0.0	0.0	1.0	0.0	0.0	1.0
LYS	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0
LYS	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	0	1	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0
MET	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PHE	1	0	0	0	0	0	1	0	0	1	2	0	0	1	1	0	0	0	0	0
PHE	2.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	3.0	5.5	0.0	0.0	5.0	5.0	0.0	0.0	0.0	0.0	0.0
PRO	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
PRO	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	12.0	0.0
SER	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SER	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
THR	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	0	0	0	0	0	1	0	0	0	2	1	0	0	2	0	0	2	2	0	0
VAL	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.5	1.0	0.0	0.0	3.5	0.0	0.0	2.5	1.0	0.0	0.0

Table 93: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between α -helices and β -sheets with crossing angles between -150° and -120° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	1	0	0	0	0	0	0	0	0	0	3	0	0	0	2	0	0	1	0	0
ALA	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0
ARG	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
GLU	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	3	0	0	0	1	0	4	0	0	0	3	3	2	2	0	0	0	0	2	1
ILE	1.3	0.0	0.0	0.0	2.0	0.0	1.5	0.0	0.0	0.0	1.3	2.7	3.0	2.5	0.0	0.0	0.0	0.0	2.5	1.0
LEU	2	0	0	0	0	0	0	0	0	0	4	0	0	1	0	0	2	2	1	0
LEU	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	4.0	0.0	0.0	1.0	1.5	4.0	0.0
LYS	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
LYS	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	11.0	0.0	0.0
MET	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	7.0	0.0	0.0
PHE	2	0	0	0	0	0	0	0	0	1	4	0	1	1	0	0	1	0	0	2
PHE	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	2.0	0.0	6.0	3.0	0.0	0.0	3.0	0.0	0.0	3.5
PRO	1	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0
PRO	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0
SER	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
SER	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRP	1	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	0	1
TRP	6.0	12.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.5	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	3.0	1.0
TYR	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
TYR	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
VAL	3	0	0	0	1	0	1	0	0	1	4	0	0	0	0	2	1	0	1	4
VAL	1.3	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	1.2	0.0	0.0	0.0	0.0	1.0	2.0	0.0	2.0	1.2

Table 94: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between α -helices and β -sheets with crossing angles between -180° and -150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	2
ALA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
CYS	0.0	2.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
GLN	0	0	0	0	0	1	0	0	0	0	0	0	1	0	1	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
GLU	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	4	2	0	0	0	0	0	0	0	0	1	1	0	0	0	0	1	0	0	0
ILE	1.2	5.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	4.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
LEU	2	0	0	0	0	0	0	0	0	1	4	1	0	0	0	0	0	0	0	2
LEU	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.5	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0
LYS	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	0	1	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	1
MET	0.0	3.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
PHE	1	0	0	0	0	0	1	0	0	0	1	0	0	1	0	0	0	2	0	0
PHE	2.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	1.0	0.0	0.0	3.0	0.0	0.0	0.0	4.0	0.0	0.0
PRO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	1	1	0	0	0	3	0	0	0	1	2	0	0	0	0	0	1	0	0	1
THR	1.0	2.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0
TRP	0	0	0	1	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	1
TRP	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	5.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
TYR	0	0	0	0	0	0	0	0	1	1	0	0	0	1	0	0	0	0	0	0
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	13.0	7.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
VAL	2	0	0	0	0	2	0	0	0	0	2	0	3	2	0	1	0	1	1	3
VAL	1.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	3.0	0.0	1.7	3.5	0.0	1.0	0.0	4.0	2.0	1.7

Table 95: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of β -sheets with crossing angles between 0° and 30° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	1	0	0	1	0	0	0	1	1	0	0	0	0	0
ALA	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	1.0	0.0	0.0	0.0	4.0	1.0	0.0	0.0	0.0	0.0	0.0
ARG	0	0	0	0	0	1	0	0	0	0	2	0	0	0	0	0	0	0	2	0
ARG	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	1	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
ASP	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
GLN	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLN	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
GLU	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	0	0	0	1	0	0	0	0	0	2	1	0	1	0	0	0	0	0	0	2
ILE	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	3.0	2.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5
LEU	0	2	2	0	0	0	0	0	0	1	2	1	0	2	1	0	0	0	0	2
LEU	0.0	2.5	2.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	1.0	0.0	4.0	1.0	0.0	0.0	0.0	0.0	2.0
LYS	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
LYS	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0
PHE	1	0	0	0	0	0	1	0	0	0	2	0	0	0	0	0	0	0	1	2
PHE	4.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	5.5
PRO	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0
PRO	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
THR	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	2	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0
TYR	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0
VAL	0	0	0	0	0	0	0	0	0	2	2	0	1	2	0	0	1	0	0	8
VAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	2.0	0.0	2.0	5.5	0.0	0.0	1.0	0.0	0.0	1.0

Table 96: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of β -sheets with crossing angles between 30° and 60° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	0	0	0	0	0	0	2	0	1	0	0	0	0	1
ALA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	3.0	0.0	0.0	0.0	0.0	1.0
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
ASP	0	0	0	0	1	0	0	0	1	0	2	0	0	0	0	0	1	0	1	0
ASP	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	3.0	0.0
CYS	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
CYS	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLU	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	0	0	0	0	1	0	0	0	0	0	2	0	1	1	0	0	1	0	0	10
ILE	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	2.5	0.0	1.0	1.0	0.0	0.0	2.0	0.0	0.0	1.4
LEU	0	0	1	2	0	1	0	0	0	2	3	0	0	3	0	0	1	0	1	2
LEU	0.0	0.0	2.0	1.0	0.0	1.0	0.0	0.0	0.0	2.5	1.3	0.0	0.0	2.3	0.0	0.0	1.0	0.0	10.0	1.0
LYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	2	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	2
MET	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	2.0
PHE	0	0	0	0	0	0	0	0	0	1	3	0	1	0	0	0	2	0	0	1
PHE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.3	0.0	4.0	0.0	0.0	0.0	1.0	0.0	0.0	6.0
PRO	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PRO	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
THR	0	0	1	1	0	0	0	0	0	1	1	0	0	2	0	2	0	0	3	0
THR	0.0	0.0	1.0	2.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	2.3	0.0
TRP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TYR	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	3	0	0	2
TYR	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	10.0	0.0	0.0	0.0	0.0	0.0	2.3	0.0	0.0	1.5
VAL	1	0	0	0	0	0	0	0	0	10	2	0	2	1	0	0	0	0	2	8
VAL	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.4	1.0	0.0	2.0	6.0	0.0	0.0	0.0	0.0	1.5	1.2

Table 97: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of β -sheets with crossing angles between 60° and 90° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	0	0	0	1	6	0	0	1	0	0	2	0	0	3
ALA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.5	0.0	0.0	3.0	0.0	0.0	2.0	0.0	0.0	1.3
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5
ASP	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	0	1	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	0.0	0.0	2.0	0.0	0.0	0.0	3.0	0.0	0.0
CYS	0	0	0	0	0	1	0	0	0	0	1	1	1	1	0	0	0	0	0	1
CYS	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	1.0	5.0	4.0	2.0	0.0	0.0	0.0	0.0	0.0	2.0
GLN	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
GLN	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
GLU	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	1	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	4.0	2.0	0.0	0.0
ILE	1	0	0	1	0	0	0	0	0	6	7	0	1	3	1	0	0	0	1	3
ILE	1.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	2.0	1.7	0.0	2.0	3.7	1.0	0.0	0.0	0.0	1.0	2.3
LEU	6	0	0	1	1	0	0	0	0	7	10	0	2	7	2	0	3	1	2	10
LEU	1.5	0.0	0.0	2.0	1.0	0.0	0.0	0.0	0.0	1.7	1.4	0.0	1.5	2.6	1.0	0.0	1.0	2.0	1.5	1.3
LYS	0	0	0	0	1	0	0	0	1	0	0	0	0	1	0	1	0	0	0	0
LYS	0.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	14.0	0.0	2.0	0.0	0.0	0.0	0.0
MET	0	0	0	0	1	0	0	0	0	1	2	0	0	1	0	0	0	0	0	0
MET	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	2.0	1.5	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
PHE	1	0	0	1	1	0	0	0	0	3	7	1	1	0	1	0	0	0	2	2
PHE	3.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	0.0	3.7	2.6	14.0	2.0	0.0	10.0	0.0	0.0	0.0	4.5	1.0
PRO	0	0	0	0	0	0	0	0	0	1	2	0	0	1	0	1	0	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	10.0	0.0	2.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0
THR	2	0	0	0	0	1	0	0	1	0	3	0	0	0	0	0	0	0	0	3
THR	2.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	4.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.7
TRP	0	0	0	1	0	0	0	0	1	0	1	0	0	0	0	0	0	2	0	2
TRP	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	2.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	0.0	1.5
TYR	0	0	0	0	0	0	0	0	0	1	2	0	0	2	0	0	0	0	0	2
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.5	0.0	0.0	4.5	0.0	0.0	0.0	0.0	0.0	1.0
VAL	3	0	2	0	1	0	0	0	0	3	10	0	0	2	0	0	3	2	2	0
VAL	1.3	0.0	1.5	0.0	2.0	0.0	0.0	0.0	0.0	2.3	1.3	0.0	0.0	1.0	0.0	0.0	1.7	1.5	1.0	0.0

Table 98: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of β -sheets with crossing angles between 90° and 120° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	0	0	0	1	6	0	0	1	0	0	2	0	0	3
ALA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.5	0.0	0.0	3.0	0.0	0.0	2.0	0.0	0.0	1.3
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5
ASP	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	0	1	0	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	0.0	0.0	2.0	0.0	0.0	0.0	3.0	0.0	0.0
CYS	0	0	0	0	0	1	0	0	0	0	1	1	1	1	0	0	0	0	0	1
CYS	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	1.0	5.0	4.0	2.0	0.0	0.0	0.0	0.0	0.0	2.0
GLN	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
GLN	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
GLU	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	1	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	4.0	2.0	0.0	0.0
ILE	1	0	0	1	0	0	0	0	0	6	7	0	1	3	1	0	0	0	1	3
ILE	1.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	2.0	1.7	0.0	2.0	3.7	1.0	0.0	0.0	0.0	1.0	2.3
LEU	6	0	0	1	1	0	0	0	0	7	10	0	2	7	2	0	3	1	2	10
LEU	1.5	0.0	0.0	2.0	1.0	0.0	0.0	0.0	0.0	1.7	1.4	0.0	1.5	2.6	1.0	0.0	1.0	2.0	1.5	1.3
LYS	0	0	0	0	1	0	0	0	1	0	0	0	0	1	0	1	0	0	0	0
LYS	0.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	14.0	0.0	2.0	0.0	0.0	0.0	0.0
MET	0	0	0	0	1	0	0	0	0	1	2	0	0	1	0	0	0	0	0	0
MET	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	2.0	1.5	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
PHE	1	0	0	1	1	0	0	0	0	3	7	1	1	0	1	0	0	0	2	2
PHE	3.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	0.0	3.7	2.6	14.0	2.0	0.0	10.0	0.0	0.0	0.0	4.5	1.0
PRO	0	0	0	0	0	0	0	0	0	1	2	0	0	1	0	1	0	0	0	0
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	10.0	0.0	2.0	0.0	0.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0
THR	2	0	0	0	0	1	0	0	1	0	3	0	0	0	0	0	0	0	0	3
THR	2.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	4.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.7
TRP	0	0	0	1	0	0	0	0	1	0	1	0	0	0	0	0	0	0	2	2
TRP	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	2.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	0.0	1.5
TYR	0	0	0	0	0	0	0	0	0	1	2	0	0	2	0	0	0	0	0	2
TYR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.5	0.0	0.0	4.5	0.0	0.0	0.0	0.0	0.0	1.0
VAL	3	0	2	0	1	0	0	0	0	3	10	0	0	2	0	0	3	2	2	0
VAL	1.3	0.0	1.5	0.0	2.0	0.0	0.0	0.0	0.0	2.3	1.3	0.0	0.0	1.0	0.0	0.0	1.7	1.5	1.0	0.0

Table 99: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of β -sheets with crossing angles between 120° and 150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	4	1	0	0	0	0	0	0	2	9	4	2	0	6	1	2	3	1	9	12
ALA	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.4	1.5	1.5	0.0	1.8	3.0	1.0	1.0	1.0	1.6	1.2
ARG	1	0	0	0	0	1	1	0	0	2	0	0	1	3	0	1	0	3	1	0
ARG	1.0	0.0	0.0	0.0	0.0	3.0	3.0	0.0	0.0	4.0	0.0	0.0	2.0	4.0	0.0	2.0	0.0	3.3	4.0	0.0
ASN	0	0	0	1	0	1	3	0	0	3	0	2	0	0	0	0	0	1	4	2
ASN	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	1.3	0.0	3.0	0.0	0.0	0.0	0.0	0.0	1.0	2.8	1.5
ASP	0	0	1	0	0	0	3	0	0	2	0	2	0	0	0	1	1	1	4	0
ASP	0.0	0.0	1.0	0.0	0.0	0.0	1.7	0.0	0.0	2.5	0.0	2.0	0.0	0.0	0.0	1.0	1.0	3.0	1.8	0.0
CYS	0	0	0	0	2	0	0	0	1	1	2	2	1	2	1	0	2	0	1	4
CYS	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	1.0	1.0	3.0	2.0	1.0	1.0	1.0	0.0	2.0	0.0	4.0	1.0
GLN	0	1	1	0	0	0	0	0	2	2	2	1	0	0	0	0	0	0	2	4
GLN	0.0	3.0	1.0	0.0	0.0	0.0	0.0	0.0	2.5	1.5	3.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	1.8
GLU	0	1	3	3	0	0	0	0	0	1	2	4	0	0	1	1	5	0	5	4
GLU	0.0	3.0	1.0	1.7	0.0	0.0	0.0	0.0	0.0	3.0	2.0	3.0	0.0	0.0	1.0	1.0	1.6	0.0	2.4	3.2
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	2	0	0	0	1	2	0	0	10	1	4	0	2	2	0	1	0	3	3	2
HIS	2.0	0.0	0.0	0.0	1.0	2.5	0.0	0.0	1.2	1.0	2.2	0.0	3.0	1.0	0.0	1.0	0.0	6.0	2.7	2.0
ILE	9	2	3	2	1	2	1	0	1	14	9	2	2	11	1	2	4	5	5	10
ILE	1.4	4.0	1.3	2.5	1.0	1.5	3.0	0.0	1.0	2.0	1.4	3.5	3.5	2.7	1.0	1.0	2.2	2.8	1.2	2.0
LEU	4	0	0	0	2	2	2	0	4	9	10	1	6	16	0	2	3	1	5	25
LEU	1.5	0.0	0.0	0.0	1.0	3.0	2.0	0.0	2.2	1.4	2.4	8.0	2.2	2.6	0.0	1.5	1.3	4.0	2.4	1.9
LYS	2	0	2	2	2	1	4	0	0	2	1	0	0	1	0	3	5	1	2	4
LYS	1.5	0.0	3.0	2.0	3.0	2.0	3.0	0.0	0.0	3.5	8.0	0.0	0.0	3.0	0.0	2.0	1.4	14.0	2.0	1.8
MET	0	1	0	0	1	0	0	0	2	2	6	0	0	3	2	1	1	0	3	5
MET	0.0	2.0	0.0	0.0	2.0	0.0	0.0	0.0	3.0	3.5	2.2	0.0	0.0	7.7	1.5	2.0	3.0	0.0	2.7	3.4
PHE	6	3	0	0	2	0	0	0	2	11	16	1	3	16	0	1	3	4	2	11
PHE	1.8	4.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	2.7	2.6	3.0	7.7	3.5	0.0	3.0	2.3	6.2	3.0	2.1
PRO	1	0	0	0	1	0	1	0	0	1	0	0	2	0	0	0	0	0	0	7
PRO	3.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	1.6
SER	2	1	0	1	0	0	1	0	1	2	2	3	1	1	0	2	4	0	0	6
SER	1.0	2.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	1.0	1.5	2.0	2.0	3.0	0.0	1.0	1.2	0.0	0.0	1.0
THR	3	0	0	1	2	0	5	0	0	4	3	5	1	3	0	4	2	2	4	2
THR	1.0	0.0	0.0	1.0	2.0	0.0	1.6	0.0	0.0	2.2	1.3	1.4	3.0	2.3	0.0	1.2	1.0	2.5	2.8	1.5
TRP	1	3	1	1	0	0	0	0	3	5	1	1	0	4	0	0	2	0	0	3
TRP	1.0	3.3	1.0	3.0	0.0	0.0	0.0	0.0	6.0	2.8	4.0	14.0	0.0	6.2	0.0	0.0	2.5	0.0	0.0	8.3
TYR	9	1	4	4	1	2	5	0	3	5	5	2	3	2	0	0	4	0	8	4
TYR	1.6	4.0	2.8	1.8	4.0	1.5	2.4	0.0	2.7	1.2	2.4	2.0	2.7	3.0	0.0	0.0	2.8	0.0	5.0	3.8
VAL	12	0	2	0	4	4	4	0	2	10	25	4	5	11	7	6	2	3	4	28
VAL	1.2	0.0	1.5	0.0	1.0	1.8	3.2	0.0	2.0	2.0	1.9	1.8	3.4	2.1	1.6	1.0	1.5	8.3	3.8	1.6

Table 100: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of β -sheets with crossing angles between 150° and 180° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	1	1	2	0	1	5	7	1	2	4	3	0	3	2	5	12
ALA	0.0	0.0	0.0	0.0	1.0	2.0	1.0	0.0	1.0	1.2	1.4	1.0	1.5	2.0	1.7	0.0	1.0	1.5	2.0	1.1
ARG	0	0	0	1	0	1	1	0	0	2	4	0	0	2	0	1	3	0	6	0
ARG	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	2.0	1.5	0.0	0.0	2.5	0.0	2.0	1.7	0.0	2.7	0.0
ASN	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	2	0	1	4
ASN	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	4.0	1.0
ASP	0	1	0	0	0	2	1	0	0	2	2	0	0	2	0	0	0	0	1	1
ASP	0.0	1.0	0.0	0.0	0.0	1.0	2.0	0.0	0.0	1.0	1.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	2.0	1.0
CYS	1	0	0	0	4	0	1	0	1	1	6	0	3	4	0	1	0	2	1	0
CYS	1.0	0.0	0.0	0.0	4.0	0.0	2.0	0.0	3.0	1.0	2.3	0.0	4.0	1.8	0.0	1.0	0.0	3.5	4.0	0.0
GLN	1	1	0	2	0	0	0	0	1	2	1	2	0	1	0	0	2	0	2	7
GLN	2.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	2.0	2.0	1.5	0.0	1.0	0.0	0.0	1.0	0.0	2.5	1.9
GLU	2	1	2	1	1	0	0	0	0	4	5	4	0	0	1	1	3	0	0	1
GLU	1.0	1.0	1.0	2.0	2.0	0.0	0.0	0.0	0.0	1.2	2.0	2.5	0.0	0.0	2.0	1.0	2.3	0.0	0.0	3.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	1	0	0	0	1	1	0	0	0	1	0	0	1	0	0	1	0	0	1	3
HIS	1.0	0.0	0.0	0.0	3.0	1.0	0.0	0.0	0.0	2.0	0.0	0.0	2.0	0.0	0.0	1.0	0.0	0.0	1.0	2.0
ILE	5	2	0	2	1	2	4	0	1	6	18	5	1	4	2	3	5	0	6	16
ILE	1.2	2.0	0.0	1.0	1.0	2.0	1.2	0.0	2.0	2.7	1.9	1.6	2.0	2.8	2.5	1.3	1.6	0.0	2.7	1.6
LEU	7	4	0	2	6	1	5	0	0	15	26	3	7	6	7	0	8	6	5	24
LEU	1.4	1.5	0.0	1.0	2.3	2.0	2.0	0.0	0.0	2.0	2.0	2.3	2.1	2.7	1.6	0.0	2.1	2.7	3.0	2.3
LYS	1	0	0	0	0	2	4	0	0	5	3	0	0	4	0	1	3	1	1	1
LYS	1.0	0.0	0.0	0.0	0.0	1.5	2.5	0.0	0.0	1.6	2.3	0.0	0.0	2.5	0.0	3.0	2.3	9.0	4.0	1.0
MET	2	0	0	0	3	0	0	0	1	1	7	0	2	5	0	0	1	0	0	2
MET	1.5	0.0	0.0	0.0	4.0	0.0	0.0	0.0	2.0	2.0	2.1	0.0	1.0	4.4	0.0	0.0	1.0	0.0	0.0	1.5
PHE	4	2	0	2	4	1	0	0	0	4	6	4	5	10	0	1	2	1	5	11
PHE	2.0	2.5	0.0	3.0	1.8	1.0	0.0	0.0	0.0	2.8	2.7	2.5	4.4	4.4	0.0	6.0	2.0	1.0	2.8	2.3
PRO	1	0	0	0	0	0	1	0	0	1	7	0	0	0	0	1	2	1	1	5
PRO	1.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	4.0	1.6	0.0	0.0	0.0	0.0	1.0	1.0	1.0	6.0	1.4
SER	0	1	0	0	1	0	1	0	1	3	0	1	0	1	1	4	4	0	4	4
SER	0.0	2.0	0.0	0.0	1.0	0.0	1.0	0.0	1.0	1.3	0.0	3.0	0.0	6.0	1.0	1.0	1.0	0.0	2.2	1.0
THR	3	3	2	0	0	2	3	0	0	5	8	3	1	2	2	4	4	0	5	4
THR	1.0	1.7	1.0	0.0	0.0	1.0	2.3	0.0	0.0	1.6	2.1	2.3	1.0	2.0	1.0	1.0	2.0	0.0	1.4	1.2
TRP	2	0	0	0	2	0	0	0	0	0	6	1	0	1	1	0	0	0	2	1
TRP	1.5	0.0	0.0	0.0	3.5	0.0	0.0	0.0	0.0	0.0	2.7	9.0	0.0	1.0	1.0	0.0	0.0	0.0	6.0	1.0
TYR	5	6	1	1	1	2	0	0	1	6	5	1	0	5	1	4	5	2	4	13
TYR	2.0	2.7	4.0	2.0	4.0	2.5	0.0	0.0	1.0	2.7	3.0	4.0	0.0	2.8	6.0	2.2	1.4	6.0	4.5	2.6
VAL	11	0	4	1	0	7	1	0	2	15	24	1	2	11	4	4	4	1	13	16
VAL	1.1	0.0	1.0	1.0	0.0	1.9	3.0	0.0	2.5	1.7	2.3	1.0	1.5	2.3	1.5	1.0	1.2	1.0	2.6	1.6

Table 101: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of β -sheets with crossing angles between -30° and 0° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	1	1	0	0	0	5	4	1	2	2	0	1	0	1	4	8
ALA	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	1.0	1.2	1.0	1.0	2.5	0.0	1.0	0.0	3.0	2.0	1.2
ARG	0	0	0	0	0	0	0	0	0	2	1	1	0	1	0	0	0	0	2	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	1.0	0.0	2.0	0.0	0.0	0.0	0.0	2.5	0.0
ASN	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	1	0	1	0	0	0	1	0	0	0	0	0	0	0	0	1
ASP	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
CYS	1	0	0	1	0	1	0	0	0	0	0	1	0	1	0	0	0	0	0	2
CYS	1.0	0.0	0.0	1.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	1.0
GLN	1	0	0	0	1	0	1	0	0	1	0	0	0	1	0	0	2	0	0	0
GLN	1.0	0.0	0.0	0.0	2.0	0.0	2.0	0.0	0.0	1.0	0.0	0.0	0.0	4.0	0.0	0.0	1.0	0.0	0.0	0.0
GLU	0	0	0	1	0	1	0	0	0	1	0	0	0	0	0	1	0	0	0	0
GLU	0.0	0.0	0.0	1.0	0.0	2.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	6	2	0	0	0	1	1	0	1	14	14	1	2	5	0	0	1	2	0	14
ILE	1.0	2.0	0.0	0.0	0.0	1.0	3.0	0.0	1.0	2.1	2.4	4.0	3.0	2.2	0.0	0.0	2.0	3.0	0.0	1.7
LEU	4	1	1	1	0	0	0	0	0	14	18	1	8	5	1	0	2	1	1	18
LEU	1.2	2.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	2.4	1.9	1.0	2.0	2.0	3.0	0.0	2.5	3.0	2.0	1.8
LYS	1	1	0	0	1	0	0	0	0	1	1	0	1	0	1	3	2	0	2	1
LYS	1.0	1.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	4.0	1.0	0.0	1.0	0.0	4.0	1.0	4.0	0.0	2.5	2.0
MET	2	0	0	0	0	0	0	0	0	2	6	1	0	2	1	0	0	2	0	5
MET	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	2.0	1.0	0.0	1.5	3.0	0.0	0.0	7.0	0.0	1.0
PHE	2	1	0	0	1	1	0	0	0	5	5	0	2	4	0	0	0	0	3	10
PHE	2.5	2.0	0.0	0.0	4.0	4.0	0.0	0.0	0.0	2.2	2.0	0.0	1.5	2.0	0.0	0.0	0.0	0.0	4.7	2.7
PRO	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	1
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	4.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0
SER	1	0	0	0	0	0	1	0	0	0	0	3	0	0	0	0	0	0	1	0
SER	1.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
THR	0	0	0	0	0	2	0	0	0	1	2	2	0	0	0	0	0	1	0	0
THR	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	2.0	2.5	4.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0
TRP	1	0	0	0	0	0	0	0	0	2	1	0	2	0	0	0	1	0	0	2
TRP	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	3.0	0.0	7.0	0.0	0.0	0.0	2.0	0.0	0.0	3.5
TYR	4	2	0	0	0	0	0	0	0	1	2	0	3	0	1	0	0	0	0	4
TYR	2.0	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.5	0.0	4.7	0.0	1.0	0.0	0.0	0.0	0.0	1.5
VAL	8	0	0	1	2	0	0	0	0	14	18	1	5	10	1	0	0	2	4	38
VAL	1.2	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	1.7	1.8	2.0	1.0	2.7	3.0	0.0	0.0	3.5	1.5	2.2

Table 102: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of β -sheets with crossing angles between -60° and -30° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	2	0	0	0	0	0	0	0	0	4	3	0	0	2	1	0	1	1	0	4
ALA	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	1.5	1.0	0.0	1.0	1.0	0.0	1.0
ARG	0	0	0	1	0	0	1	0	0	1	0	1	0	0	0	0	0	0	0	1
ARG	0.0	0.0	0.0	3.0	0.0	0.0	1.0	0.0	0.0	4.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
ASN	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	1	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	1	0
ASP	0.0	3.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
CYS	0	0	0	0	2	0	0	0	0	1	1	0	1	1	0	1	0	0	0	1
CYS	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	2.0	8.0	0.0	1.0	0.0	0.0	0.0	2.0
GLN	0	0	0	1	0	0	1	0	0	1	1	0	0	1	0	0	0	2	0	2
GLN	0.0	0.0	0.0	2.0	0.0	0.0	1.0	0.0	0.0	1.0	5.0	0.0	0.0	5.0	0.0	0.0	0.0	1.5	0.0	2.5
GLU	0	1	0	0	0	1	0	0	0	1	0	1	0	1	0	0	0	0	1	0
GLU	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	2.0	0.0	2.0	0.0	0.0	0.0	0.0	1.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	4	1	0	1	1	1	1	0	0	6	11	2	1	3	2	0	2	0	5	6
ILE	1.0	4.0	0.0	1.0	1.0	1.0	1.0	0.0	0.0	2.0	1.8	3.0	1.0	4.0	2.5	0.0	1.5	0.0	2.0	1.8
LEU	3	0	1	0	1	1	0	0	0	11	13	0	0	4	0	0	1	1	0	10
LEU	1.0	0.0	1.0	0.0	1.0	5.0	0.0	0.0	0.0	1.8	1.8	0.0	0.0	1.2	0.0	0.0	1.0	7.0	0.0	1.7
LYS	0	1	0	0	0	0	1	0	1	2	0	0	0	0	0	0	2	2	1	0
LYS	0.0	2.0	0.0	0.0	0.0	0.0	2.0	0.0	1.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.0	5.0	0.0
MET	0	0	0	0	1	0	0	0	1	1	0	0	0	2	0	0	0	0	0	1
MET	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	5.0	1.0	0.0	0.0	0.0	3.5	0.0	0.0	0.0	0.0	0.0	2.0
PHE	2	0	0	0	1	1	1	0	0	3	4	0	2	0	1	1	2	0	1	10
PHE	1.5	0.0	0.0	0.0	8.0	5.0	2.0	0.0	0.0	4.0	1.2	0.0	3.5	0.0	2.0	2.0	2.0	0.0	1.0	1.8
PRO	1	0	0	0	0	0	0	0	0	2	0	0	0	1	0	0	0	2	0	2
PRO	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	0.0	0.0	0.0	2.0	0.0	0.0	0.0	10.0	0.0	1.5
SER	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	1	1	0
SER	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	2.0	1.0	0.0
THR	1	0	0	0	0	0	0	0	0	2	1	2	0	2	0	0	0	0	0	2
THR	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	1.0	1.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	1.0
TRP	1	0	0	0	0	2	0	0	0	0	1	2	0	0	2	1	0	0	1	1
TRP	1.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	7.0	2.0	0.0	0.0	10.0	2.0	0.0	0.0	2.0	6.0	6.0
TYR	0	0	0	1	0	0	1	0	0	5	0	1	0	1	0	1	0	1	2	4
TYR	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	2.0	0.0	5.0	0.0	1.0	0.0	1.0	0.0	2.0	1.0	2.2
VAL	4	1	0	0	1	2	0	0	0	6	10	0	1	10	2	0	2	1	4	16
VAL	1.0	1.0	0.0	0.0	2.0	2.5	0.0	0.0	0.0	1.8	1.7	0.0	2.0	1.8	1.5	0.0	1.0	6.0	2.2	1.6

Table 103: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of β -sheets with crossing angles between -90° and -60° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	0	0	0	4	6	0	0	0	0	1	0	5	2	1
ALA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	1.2	0.0	0.0	0.0	0.0	1.0	0.0	1.6	4.0	1.0
ARG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASN	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	0	0	1	0	1	0	0	0	3	0	0	1	0	0	0	1	0	0
ASP	0.0	0.0	0.0	0.0	2.0	0.0	2.0	0.0	0.0	0.0	1.7	0.0	0.0	2.0	0.0	0.0	0.0	1.0	0.0	0.0
CYS	0	0	0	1	0	0	0	0	0	0	4	0	0	0	0	1	0	0	0	0
CYS	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
GLN	0	0	0	0	0	0	0	0	0	1	3	0	0	0	0	0	0	2	0	0
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.3	0.0	0.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0
GLU	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	2	1	0
GLU	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.5	1.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	2	0	0	2	0	0	0	0	0	1
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	1.0
ILE	4	0	0	0	0	1	0	0	0	4	11	0	0	5	2	1	0	3	2	4
ILE	1.5	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.5	2.1	0.0	0.0	3.2	1.5	1.0	0.0	2.0	1.5	1.5
LEU	6	0	1	3	4	3	0	0	2	11	20	0	0	12	0	0	3	2	3	13
LEU	1.2	0.0	1.0	1.7	1.5	1.3	0.0	0.0	1.5	2.1	1.8	0.0	0.0	2.0	0.0	0.0	2.0	4.0	4.0	1.4
LYS	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MET	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0
PHE	0	0	0	1	0	0	0	0	2	5	12	0	2	2	0	0	0	3	0	3
PHE	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	3.0	3.2	2.0	0.0	3.0	2.0	0.0	0.0	0.0	1.7	0.0	1.7
PRO	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	0	1
PRO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	3.0
SER	1	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
SER	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	1
THR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
TRP	5	0	0	1	0	2	2	0	0	3	2	0	0	3	1	0	0	0	0	2
TRP	1.6	0.0	0.0	1.0	0.0	5.0	3.5	0.0	0.0	2.0	4.0	0.0	0.0	1.7	1.0	0.0	0.0	0.0	0.0	3.0
TYR	2	0	0	0	0	0	1	0	0	2	3	0	0	0	0	0	0	0	2	0
TYR	4.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.5	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0
VAL	1	0	0	0	0	0	0	0	1	4	13	0	0	3	1	0	1	2	0	16
VAL	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.5	1.4	0.0	0.0	1.7	3.0	0.0	1.0	3.0	0.0	1.8

Table 104: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of β -sheets with crossing angles between -120° and -90° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	1	0	0	0	4	2	1	0	2	0	2	1	0	0	0
ALA	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	2.0	1.0	0.0	1.5	0.0	1.0	2.0	0.0	0.0	0.0
ARG	0	0	0	0	0	0	0	0	0	0	0	0	1	0	2	0	0	0	0	2
ARG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	3.5	0.0	0.0	0.0	0.0	4.0
ASN	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	1
ASN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0
ASP	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	1	0
ASP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0
CYS	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0
GLN	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1
GLN	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
GLU	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	1
GLU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	4	0	0	4	0	0	0	0	0	2	2	0	0	2	1	2	0	2	2	5
ILE	1.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0	1.0	2.0	0.0	0.0	1.0	2.0	1.0	0.0	3.5	2.0	2.2
LEU	2	0	2	0	1	1	2	0	0	2	20	0	0	5	1	0	2	1	1	4
LEU	2.0	0.0	1.0	0.0	2.0	1.0	1.0	0.0	0.0	2.0	1.4	0.0	0.0	2.0	1.0	0.0	1.0	3.0	8.0	1.8
LYS	1	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	1	1	1	1
LYS	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	1.0	4.0	4.0	1.0
MET	0	1	0	0	0	0	0	0	0	0	0	0	2	4	0	0	2	0	1	0
MET	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	1.0	0.0	0.0	1.5	0.0	1.0	12.0	0.0
PHE	2	0	0	0	0	0	0	0	0	2	5	0	0	4	0	2	3	1	0	2
PHE	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.0	0.0	0.0	1.0	0.0	3.0	1.7	5.0	0.0	2.0
PRO	0	2	0	0	0	0	0	0	0	1	1	0	0	0	0	0	1	0	0	0
PRO	0.0	3.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0
SER	2	0	0	0	0	0	0	0	0	2	0	0	2	2	0	0	0	0	0	0
SER	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.5	3.0	0.0	0.0	0.0	0.0	0.0	0.0
THR	1	0	0	0	0	0	0	0	0	0	2	1	0	3	1	0	0	0	2	1
THR	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	1.7	1.0	0.0	0.0	0.0	4.5	1.0
TRP	0	0	0	0	0	0	0	0	0	2	1	1	1	1	0	0	0	4	0	1
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.5	3.0	4.0	1.0	5.0	0.0	0.0	0.0	6.5	0.0	3.0
TYR	0	0	0	1	0	0	0	0	0	2	1	1	1	0	0	0	2	0	0	0
TYR	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	2.0	8.0	4.0	12.0	0.0	0.0	0.0	4.5	0.0	0.0	0.0
VAL	0	2	1	0	1	1	1	0	0	5	4	1	0	2	0	0	1	1	0	4
VAL	0.0	4.0	2.0	0.0	4.0	1.0	1.0	0.0	0.0	2.2	1.8	1.0	0.0	2.0	0.0	0.0	1.0	3.0	0.0	1.0

Table 105: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of β -sheets with crossing angles between -150° and -120° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	1	0	1	2
ALA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	2.0	1.5
ARG	0	0	0	0	0	0	1	0	0	2	0	0	0	0	0	0	0	0	0	1
ARG	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
ASN	0	0	0	1	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	1
ASP	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0
CYS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0
GLN	0	0	0	0	0	0	0	0	1	0	2	0	0	0	1	0	0	0	1	1
GLN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	1.5	0.0	0.0	0.0	1.0	0.0	0.0	0.0	8.0	1.0
GLU	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0
GLU	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	0	1	0	0	2	1	0	0	0	0	0	0	0	0	0	0
HIS	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ILE	2	2	1	1	0	0	0	0	1	2	5	1	1	3	0	1	1	1	2	2
ILE	1.5	2.5	1.0	1.0	0.0	0.0	0.0	1.0	2.0	2.2	3.0	1.0	5.3	0.0	1.0	1.0	1.0	2.5	1.0	
LEU	0	0	0	0	0	2	0	0	0	5	8	0	0	7	0	2	0	2	3	5
LEU	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	2.2	2.2	0.0	0.0	2.9	0.0	1.0	0.0	4.5	3.0	1.6
LYS	0	0	0	0	0	0	0	0	0	1	0	2	0	0	0	0	1	1	0	0
LYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	8.0	0.0	0.0
MET	0	0	1	0	0	0	0	0	0	1	0	0	0	0	2	0	0	1	0	1
MET	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	2.0	0.0	1.0
PHE	0	0	0	0	0	0	0	0	0	3	7	0	0	4	0	1	0	0	0	3
PHE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.3	2.9	0.0	0.0	3.5	0.0	1.0	0.0	0.0	0.0	8.3
PRO	0	0	0	0	0	1	0	0	0	0	0	0	2	0	0	0	0	2	0	0
PRO	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0
SER	0	0	0	0	0	0	0	0	0	1	2	0	0	1	0	0	0	0	0	1
SER	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0
THR	1	0	0	1	0	0	1	0	0	1	0	1	0	0	0	0	2	0	0	1
THR	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	3.0
TRP	0	0	0	0	0	0	0	0	0	1	2	1	1	0	2	0	0	2	3	2
TRP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	4.5	8.0	2.0	0.0	2.0	0.0	0.0	3.0	5.3	2.5
TYR	1	0	0	0	1	1	1	0	0	2	3	0	0	0	0	0	0	3	0	0
TYR	2.0	0.0	0.0	0.0	1.0	8.0	1.0	0.0	0.0	2.5	3.0	0.0	0.0	0.0	0.0	0.0	0.0	5.3	0.0	0.0
VAL	2	1	0	1	1	1	0	0	0	2	5	0	1	3	0	1	1	2	0	6
VAL	1.5	1.0	0.0	2.0	1.0	1.0	0.0	0.0	0.0	1.0	1.6	0.0	1.0	8.3	0.0	1.0	3.0	2.5	0.0	2.0

Table 106: Total residue-residue interactions and average atom contacts for interactions between hydrophobic side-chains. Interactions are between pairs of β -sheets with crossing angles between -180° and -150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
ALA	0	0	0	3	0	2	0	0	0	1	3	0	0	2	1	0	1	0	1	2
ALA	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	1.0	1.3	0.0	0.0	1.5	1.0	0.0	1.0	0.0	2.0	1.0
ARG	0	0	0	1	0	0	1	0	0	0	0	0	0	1	0	0	2	1	2	3
ARG	0.0	0.0	0.0	1.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	2.0	12.0	3.5	3.3
ASN	0	0	0	0	0	1	0	0	0	2	2	0	0	0	0	0	0	0	0	0
ASN	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASP	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	1
ASP	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0	1.0
CYS	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2	0
CYS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
GLN	2	0	1	0	0	0	1	0	1	0	0	0	0	1	2	0	0	0	1	1
GLN	1.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	2.0	0.0	0.0	0.0	0.0	2.0	1.0	0.0	0.0	0.0	3.0	2.0
GLU	0	1	0	0	0	1	0	0	0	2	1	3	0	0	1	1	0	0	3	2
GLU	0.0	2.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.5	1.0	2.7	0.0	0.0	2.0	1.0	0.0	0.0	3.7	4.0
GLY	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GLY	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HIS	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0	1	0	1	0
HIS	0.0	0.0	0.0	0.0	1.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	3.0	0.0	1.0	0.0
ILE	1	0	2	0	0	0	2	0	0	2	3	0	0	2	1	1	2	1	3	7
ILE	1.0	0.0	2.0	0.0	0.0	0.0	1.5	0.0	0.0	1.0	2.0	0.0	0.0	2.5	4.0	1.0	2.5	1.0	3.0	1.3
LEU	3	0	2	0	0	0	1	0	0	6	14	2	1	3	0	0	5	3	2	8
LEU	1.3	0.0	2.0	0.0	0.0	0.0	1.0	0.0	0.0	1.7	2.3	1.0	8.0	4.0	0.0	0.0	1.4	1.7	1.5	2.1
LYS	0	0	0	0	0	0	3	0	0	0	2	0	1	1	0	0	2	1	0	1
LYS	0.0	0.0	0.0	0.0	0.0	0.0	2.7	0.0	0.0	0.0	1.0	0.0	1.0	3.0	0.0	0.0	1.5	12.0	0.0	2.0
MET	0	0	0	0	0	0	0	0	0	1	1	0	1	1	1	0	0	0	0	1
MET	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.0	1.0	0.0	6.0	3.0	0.0	0.0	0.0	0.0	0.0	2.0
PHE	2	1	0	0	0	1	0	0	1	2	3	1	1	6	0	1	0	0	5	4
PHE	1.5	2.0	0.0	0.0	0.0	2.0	0.0	0.0	1.0	2.5	4.0	3.0	6.0	5.7	0.0	3.0	0.0	0.0	2.0	3.5
PRO	3	0	0	0	0	2	1	0	0	2	0	0	1	0	0	1	1	1	0	0
PRO	1.7	0.0	0.0	0.0	0.0	1.0	2.0	0.0	0.0	2.5	0.0	0.0	3.0	0.0	0.0	2.0	1.0	1.0	0.0	0.0
SER	0	0	0	1	0	0	1	0	0	1	0	0	0	1	1	2	1	0	1	1
SER	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	3.0	2.0	1.0	1.0	0.0	5.0	1.0	1.0
THR	1	2	0	0	0	0	0	0	1	2	5	2	0	0	1	1	4	0	2	2
THR	1.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	2.5	1.4	1.5	0.0	0.0	1.0	1.0	1.5	0.0	2.5	1.0
TRP	0	1	0	0	0	0	0	0	0	1	3	1	0	0	1	0	0	2	1	0
TRP	0.0	12.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.7	12.0	0.0	0.0	1.0	0.0	0.0	10.0	1.0	0.0
TYR	1	2	0	1	2	1	3	0	1	3	2	0	0	5	0	1	2	1	4	5
TYR	2.0	3.5	0.0	2.0	1.0	3.0	3.7	0.0	1.0	3.0	1.5	0.0	0.0	2.0	0.0	5.0	2.5	1.0	2.0	2.0
VAL	3	3	0	1	0	1	2	0	1	8	8	1	1	4	1	1	2	0	5	4
VAL	1.0	3.3	0.0	1.0	0.0	2.0	4.0	0.0	1.0	1.2	2.1	2.0	2.0	3.5	1.0	1.0	1.0	0.0	2.0	4.0

APPENDIX J

Table 107: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of α -helices with crossing angles between 0° and 30° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
POSITION 11	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0
POSITION 10	0	0	0	0	0	0	0	0	1	0	1	0	1	0	0	0	0	1	0	0
POSITION 9	0	0	0	0	0	2	0	0	0	0	0	2	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	1	0	0	2	0	0	0	0	0	1	0	0	0
POSITION 7	2	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0
POSITION 6	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1
POSITION 5	1	0	1	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	1	1	0	0	1	1	1	0	0	1	1	0	0	0	1	0	0	0	0
POSITION 3	2	0	0	0	0	1	0	0	1	0	1	2	0	0	0	1	1	0	0	1
POSITION 2	6	0	0	2	1	1	0	1	0	0	1	0	0	0	0	1	0	0	0	0
POSITION 1	2	1	0	2	0	1	0	0	0	0	0	1	0	0	1	1	2	2	0	2
POSITION 0	4	0	0	0	1	0	0	0	0	2	4	0	0	0	0	0	1	1	0	1
POSITION -1	4	3	2	1	0	0	0	0	0	0	0	2	0	0	1	1	0	0	0	1
POSITION -2	5	0	0	2	0	2	0	1	1	0	0	0	0	1	1	0	0	0	2	0
POSITION -3	1	0	0	2	0	0	0	2	0	1	2	0	0	0	1	0	0	0	1	3
POSITION -4	4	0	0	0	0	0	0	1	0	2	2	0	1	0	2	0	0	0	1	0
POSITION -5	2	0	0	1	0	1	4	2	0	0	1	0	0	0	0	1	0	0	0	0
POSITION -6	1	0	2	0	0	0	1	0	0	1	0	4	0	0	0	1	0	0	0	1
POSITION -7	1	1	0	0	0	0	0	0	0	2	2	0	1	0	0	0	0	0	0	2
POSITION -8	2	0	1	0	0	0	0	1	0	3	0	0	0	0	0	1	0	0	0	0
POSITION -9	1	0	1	1	0	0	1	0	0	0	0	0	0	0	0	1	2	0	1	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 108: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of α -helices with crossing angles between 30° and 60°.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	2
POSITION 11	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	2	0	0	0
POSITION 10	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	2	0	0	0	0
POSITION 9	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2
POSITION 8	0	0	0	1	0	0	0	1	0	0	0	1	0	0	0	2	0	0	0	0
POSITION 7	2	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	2
POSITION 6	1	0	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0
POSITION 5	1	0	1	0	0	0	1	0	0	0	0	0	0	0	3	1	0	0	0	0
POSITION 4	0	1	0	1	0	0	0	1	0	0	1	2	1	0	0	0	0	0	0	0
POSITION 3	2	0	0	2	0	0	0	0	0	0	1	1	0	0	0	1	0	1	0	0
POSITION 2	1	0	0	0	0	0	0	1	1	1	3	0	1	0	0	0	0	0	0	1
POSITION 1	3	0	0	1	0	0	0	0	0	0	1	2	0	1	0	2	0	0	0	2
POSITION 0	7	0	0	1	0	1	0	0	0	0	0	0	2	0	0	1	0	0	0	1
POSITION -1	1	0	2	0	0	0	0	2	2	0	4	2	0	0	0	1	1	0	0	1
POSITION -2	1	0	1	0	0	1	0	1	0	0	1	1	0	0	2	0	4	0	0	3
POSITION -3	2	0	0	0	1	1	0	0	0	1	2	0	2	0	2	0	0	1	1	2
POSITION -4	0	2	1	0	0	0	1	0	0	0	3	0	1	3	2	1	0	0	0	1
POSITION -5	1	0	0	0	0	0	1	3	1	0	4	0	0	0	1	0	0	0	0	1
POSITION -6	1	0	0	0	2	0	0	0	0	0	2	4	1	0	0	1	0	0	0	0
POSITION -7	3	0	0	0	0	0	0	1	2	0	1	2	0	0	0	0	0	0	1	0
POSITION -8	0	0	0	0	0	0	0	3	0	1	0	0	0	2	0	2	0	0	0	1
POSITION -9	3	0	1	1	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	1
POSITION -10	0	0	0	1	1	0	2	0	0	1	2	1	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	1	0	0	0	0	2	1	0	0	0	0	3	0	1
POSITION -12	1	0	0	0	0	0	0	2	0	0	0	0	0	0	2	0	0	1	0	1

Table 109: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of α -helices with crossing angles between 60° and 90° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	1	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	1	0	1	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	1	0	0	0	0	3	0	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	3	0	0	0	0	0
POSITION 2	1	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	1	0	0	0
POSITION 1	0	0	0	0	0	0	0	0	0	0	1	3	0	0	0	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	2	0	0	0
POSITION -1	0	0	0	0	0	0	0	3	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -2	1	0	0	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -3	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 110: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of α -helices with crossing angles between 90° and 120° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	4	0	1	0	0	1	1	0	0	1
POSITION 10	0	2	0	1	0	1	3	0	0	1	0	0	0	0	1	0	0	0	0	1
POSITION 9	1	2	1	3	0	0	1	3	0	1	0	1	0	0	0	0	0	0	0	2
POSITION 8	1	0	1	0	0	1	0	0	0	1	5	1	0	1	1	2	2	0	0	1
POSITION 7	0	1	0	2	0	0	0	0	0	0	9	1	0	0	2	1	1	1	1	2
POSITION 6	4	5	1	0	0	0	0	3	1	1	2	2	2	0	0	1	2	1	1	1
POSITION 5	2	1	3	0	2	1	4	2	0	1	4	5	0	0	1	2	3	0	0	1
POSITION 4	2	1	0	0	1	1	1	1	0	1	12	2	0	0	2	2	3	2	0	1
POSITION 3	4	2	0	1	1	3	1	2	1	4	5	0	0	0	3	1	0	2	1	4
POSITION 2	4	2	2	2	0	2	0	3	0	2	2	2	3	2	2	0	5	1	1	2
POSITION 1	6	2	1	1	0	1	3	1	1	1	7	2	0	2	1	5	0	1	0	5
POSITION 0	7	1	1	0	0	0	6	0	0	3	1	1	0	1	5	2	1	1	0	6
POSITION -1	5	2	3	1	0	2	3	1	3	1	3	1	1	0	1	3	1	0	2	5
POSITION -2	7	2	1	2	0	1	3	4	0	1	4	3	1	2	0	1	3	2	0	0
POSITION -3	3	2	2	4	0	0	3	1	0	0	8	3	0	0	4	1	2	1	1	1
POSITION -4	2	1	2	1	0	1	0	0	0	2	5	0	4	0	3	1	1	2	0	8
POSITION -5	2	0	0	3	0	1	0	3	1	2	3	5	1	1	1	2	0	1	0	1
POSITION -6	4	1	2	4	0	2	1	1	1	0	2	0	0	3	1	1	0	1	0	1
POSITION -7	4	0	1	0	2	0	0	1	1	1	3	0	0	0	1	2	1	0	0	3
POSITION -8	5	2	1	2	0	1	0	0	0	1	1	4	0	0	0	2	0	0	0	0
POSITION -9	6	1	0	1	0	0	0	1	0	1	3	3	1	0	0	0	0	0	0	1
POSITION -10	1	0	0	0	0	0	6	3	2	0	0	0	0	2	1	1	0	0	0	1
POSITION -11	4	0	1	0	0	1	1	0	2	1	0	0	0	1	1	0	0	0	0	2
POSITION -12	4	0	0	0	0	0	2	1	0	1	0	0	0	1	1	0	0	0	0	3

Table 111: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of α -helices with crossing angles between 120° and 150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	2	0	1	0	1	1	0	0	0	1	1	1	0	0	0	0	1	0	0	1
POSITION 11	1	0	1	0	0	1	1	0	0	1	2	0	0	1	0	0	2	0	1	1
POSITION 10	1	0	2	0	1	2	1	1	0	1	1	0	1	1	0	0	0	0	0	2
POSITION 9	6	1	1	0	0	0	1	1	0	1	0	2	1	1	0	0	0	0	0	1
POSITION 8	3	1	0	0	0	2	0	2	1	1	6	2	0	1	0	0	1	0	0	1
POSITION 7	4	0	0	1	0	0	0	0	1	5	6	3	1	0	0	1	1	1	0	2
POSITION 6	5	0	0	1	0	0	2	2	1	3	6	0	2	1	1	1	2	3	1	4
POSITION 5	4	3	1	3	0	0	0	1	0	3	7	3	0	0	5	3	1	0	0	3
POSITION 4	6	0	1	0	1	0	0	1	1	3	11	0	4	0	2	2	2	2	0	4
POSITION 3	5	7	0	1	1	1	1	1	0	3	12	1	1	0	1	1	0	1	0	6
POSITION 2	1	2	2	3	3	0	3	6	0	1	3	2	3	2	0	5	1	3	0	5
POSITION 1	5	0	2	4	0	4	0	2	1	0	10	1	0	3	3	2	1	3	0	6
POSITION 0	11	1	0	1	2	1	2	0	0	1	6	1	2	1	2	2	0	2	0	5
POSITION -1	3	1	2	1	1	3	0	9	2	0	5	1	0	1	5	1	1	2	2	2
POSITION -2	6	0	3	2	1	4	3	3	0	1	3	5	1	0	0	5	2	1	0	0
POSITION -3	3	0	3	5	0	0	7	1	0	4	4	3	0	1	0	0	0	1	0	3
POSITION -4	0	3	0	1	0	0	0	2	0	1	9	0	1	0	4	2	1	3	1	4
POSITION -5	2	2	2	3	0	0	1	5	0	1	3	3	0	0	0	2	1	4	0	1
POSITION -6	4	1	0	3	0	0	2	3	1	1	2	2	0	0	3	1	1	1	1	3
POSITION -7	2	0	4	0	0	0	0	3	1	1	0	2	1	1	2	1	3	2	0	3
POSITION -8	2	2	3	0	0	0	0	1	1	2	0	1	0	1	1	0	1	0	0	4
POSITION -9	2	0	0	0	0	0	0	3	1	1	1	0	0	4	1	0	1	0	0	2
POSITION -10	3	2	0	1	0	0	0	0	0	0	0	0	0	2	0	1	0	1	1	0
POSITION -11	0	0	0	0	0	0	1	1	0	0	1	0	0	0	0	1	0	0	0	1
POSITION -12	0	0	0	0	0	2	0	0	0	0	0	1	0	0	0	1	0	0	0	1

Table 112: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of α -helices with crossing angles between 150° and 180°.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	4	0	2	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0
POSITION 11	2	1	0	0	0	0	0	0	1	0	4	0	0	1	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	1	0	0	0	0	2	1	0	0	0	0	2	0	0	3
POSITION 9	1	0	0	0	2	0	0	0	0	1	1	1	1	0	1	0	1	0	0	1
POSITION 8	1	0	0	1	0	0	0	1	0	0	1	2	0	0	1	0	1	1	0	2
POSITION 7	1	0	0	0	1	0	0	1	0	1	5	0	1	0	2	0	0	1	0	0
POSITION 6	2	1	3	0	1	2	1	1	0	0	1	0	0	0	0	2	0	0	0	2
POSITION 5	0	2	3	2	0	2	0	1	1	1	2	0	0	0	1	1	0	1	0	1
POSITION 4	8	0	0	0	0	1	2	0	1	0	2	1	0	1	1	2	1	1	0	1
POSITION 3	6	0	0	0	2	1	0	0	0	1	9	0	1	0	1	0	1	0	0	2
POSITION 2	5	0	0	2	0	1	0	1	0	1	5	2	0	1	1	1	3	0	0	1
POSITION 1	3	2	3	1	1	1	0	2	1	3	2	2	0	0	0	0	2	1	0	2
POSITION 0	8	2	0	2	1	0	0	0	0	1	0	0	0	0	5	1	0	0	0	5
POSITION -1	3	1	4	1	0	0	1	4	1	0	1	1	1	1	1	1	2	1	0	4
POSITION -2	2	1	0	3	0	2	2	3	0	0	1	1	0	1	0	4	2	0	0	2
POSITION -3	3	0	0	2	0	0	0	1	1	1	3	1	0	3	2	0	1	1	0	2
POSITION -4	3	0	0	1	1	2	0	0	0	1	4	0	0	0	2	0	1	0	0	2
POSITION -5	1	1	1	1	0	0	2	1	0	0	0	2	0	0	3	1	0	0	0	3
POSITION -6	1	1	0	1	1	1	1	0	0	0	0	5	2	0	0	0	0	0	0	2
POSITION -7	0	1	0	1	0	2	0	0	0	1	4	1	0	1	0	0	0	0	0	1
POSITION -8	2	0	0	0	0	0	1	1	0	1	3	0	0	0	1	0	0	2	0	0
POSITION -9	3	1	1	1	0	1	0	1	0	0	1	0	0	0	0	1	1	0	0	0
POSITION -10	5	0	1	0	0	0	0	1	0	0	1	0	0	0	2	1	0	0	0	0
POSITION -11	0	0	1	1	1	3	2	0	1	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	2	0	0	1	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	3

Table 113: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of α -helices with crossing angles between -30° and 0° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	1	0	1	0	0	0	0	0	0	0	2	0	0	0	0	1	0	0	0	0
POSITION 11	1	0	0	0	0	0	0	0	0	1	4	0	0	0	0	0	0	0	1	0
POSITION 10	1	2	0	0	0	0	0	2	0	1	0	0	0	0	1	0	1	0	0	0
POSITION 9	1	0	0	0	0	0	0	1	1	0	1	2	0	0	0	1	2	0	0	0
POSITION 8	3	1	0	1	0	0	0	0	0	1	1	0	1	0	0	0	0	0	0	2
POSITION 7	1	1	0	0	0	0	1	0	0	0	5	0	1	0	0	1	1	0	0	0
POSITION 6	2	1	1	0	0	0	0	0	0	0	3	1	0	0	2	0	0	0	0	1
POSITION 5	2	3	0	0	0	0	0	0	0	1	1	0	0	0	0	2	1	0	1	1
POSITION 4	1	0	0	1	0	0	1	2	1	1	3	0	0	0	1	1	0	0	0	2
POSITION 3	4	1	0	0	0	1	0	1	0	2	1	3	0	0	1	0	1	0	0	0
POSITION 2	1	2	1	1	0	1	2	1	1	0	2	0	0	0	0	4	0	1	0	0
POSITION 1	2	1	0	1	0	1	2	1	0	3	2	0	1	1	0	0	0	1	0	1
POSITION 0	3	0	2	0	0	0	1	1	0	2	1	0	0	2	0	0	2	0	0	2
POSITION -1	2	0	0	1	0	1	1	0	0	1	5	0	0	0	0	1	2	0	0	1
POSITION -2	4	1	1	1	0	0	1	0	1	0	0	1	0	1	0	1	1	1	0	0
POSITION -3	4	0	0	1	0	1	0	2	0	0	2	0	1	0	0	1	1	0	0	1
POSITION -4	2	1	0	0	0	2	1	0	0	1	0	1	0	0	0	0	0	0	0	2
POSITION -5	2	0	0	0	0	0	3	0	0	0	0	0	1	0	0	0	1	0	0	0
POSITION -6	2	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	2
POSITION -7	0	0	0	1	0	0	0	1	0	1	2	0	0	0	0	0	0	0	0	2
POSITION -8	1	1	0	0	0	0	0	0	2	0	1	0	0	0	0	0	2	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	1	1	0	2	1	1	0	0	0	1
POSITION -10	0	0	0	0	0	1	2	1	0	0	0	0	0	0	0	2	0	0	0	0
POSITION -11	2	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0

Table 114: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of α -helices with crossing angles between -60° and -30° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	5	0	0	0	1	1	0	0	0	1	1	1	0	0	0	0	0	0	0	1
POSITION 11	1	0	2	0	0	1	0	0	0	2	2	0	1	0	0	1	2	0	1	2
POSITION 10	3	1	0	2	1	1	3	1	1	1	1	0	0	0	0	0	0	0	1	0
POSITION 9	2	1	3	0	0	2	1	2	0	0	2	3	0	2	1	0	0	0	0	3
POSITION 8	2	1	0	0	0	2	4	0	0	2	4	2	2	0	0	2	1	3	0	2
POSITION 7	9	1	0	2	0	0	1	1	0	1	4	1	1	1	2	1	2	0	1	3
POSITION 6	4	1	1	1	0	0	0	3	1	3	4	3	4	0	0	3	1	0	2	6
POSITION 5	4	1	1	3	0	2	1	2	1	3	6	4	1	1	0	4	1	1	0	4
POSITION 4	7	0	3	1	0	1	2	1	1	2	10	2	0	0	2	2	1	2	2	2
POSITION 3	6	1	1	2	0	4	0	5	0	5	6	1	2	0	2	4	1	1	1	2
POSITION 2	8	2	3	2	2	3	1	3	1	2	4	6	1	0	1	3	0	2	1	2
POSITION 1	10	1	1	3	2	1	4	2	1	6	2	4	1	1	1	0	2	5	2	1
POSITION 0	10	0	0	0	2	0	9	2	2	6	4	1	1	1	1	4	4	0	1	4
POSITION -1	9	2	0	0	1	5	3	1	2	1	7	2	3	0	1	2	3	1	0	10
POSITION -2	5	3	3	1	0	3	6	3	0	3	6	4	0	0	0	1	3	1	0	9
POSITION -3	8	4	3	1	0	1	1	0	3	3	4	2	1	3	1	0	5	0	1	6
POSITION -4	5	4	0	1	4	0	0	3	0	3	3	0	2	4	5	2	1	1	1	5
POSITION -5	2	3	0	5	2	2	2	2	3	0	2	0	1	1	1	1	2	2	0	4
POSITION -6	3	4	2	0	0	2	2	2	2	0	7	0	0	1	0	3	3	0	2	0
POSITION -7	8	1	0	0	1	1	3	3	0	1	2	0	3	0	1	1	0	1	0	4
POSITION -8	0	0	2	2	0	2	0	5	2	1	3	2	2	1	1	2	1	0	0	1
POSITION -9	1	0	1	0	0	1	5	0	1	0	2	1	0	2	1	0	3	0	0	2
POSITION -10	3	1	0	0	0	1	2	2	0	1	2	0	0	0	1	0	2	0	0	0
POSITION -11	0	0	0	0	0	0	0	1	0	0	4	0	0	1	0	0	2	2	0	2
POSITION -12	1	2	1	1	1	0	0	2	0	0	0	0	0	0	1	1	0	1	0	1

Table 115: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of α -helices with crossing angles between -90° and -60° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	1	0	0	0	0	1	0	0	2	0	0	0	1	0	0	0	0	0
POSITION 11	2	1	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
POSITION 10	0	0	2	0	0	0	0	0	1	0	1	2	0	0	0	0	0	1	0	1
POSITION 9	2	0	0	0	0	1	2	0	0	1	0	0	0	0	2	1	0	0	0	0
POSITION 8	1	0	2	0	0	2	0	0	0	0	0	1	0	0	0	0	0	0	2	2
POSITION 7	1	1	0	0	0	0	2	1	0	0	4	1	0	0	0	0	0	0	0	1
POSITION 6	5	0	0	0	0	0	0	0	0	0	1	0	0	1	1	0	1	1	0	1
POSITION 5	1	0	2	0	0	0	0	0	0	0	1	1	0	0	0	0	4	0	0	3
POSITION 4	0	0	0	1	1	0	0	0	0	1	2	2	0	0	0	0	0	0	1	6
POSITION 3	3	0	1	0	0	0	0	0	1	2	2	2	1	1	0	1	0	0	0	2
POSITION 2	0	1	2	0	0	4	1	2	0	0	1	0	0	1	0	2	0	2	0	1
POSITION 1	2	1	0	2	0	0	1	2	0	1	0	5	0	0	0	1	0	2	0	1
POSITION 0	5	2	0	0	0	1	1	2	0	2	2	0	0	0	0	1	1	0	0	2
POSITION -1	4	2	0	0	0	1	0	4	0	3	4	1	0	0	1	0	0	0	0	0
POSITION -2	1	2	1	2	0	3	0	1	0	0	2	2	0	2	0	1	1	2	0	0
POSITION -3	3	0	0	2	0	0	0	0	0	3	2	1	0	1	0	2	0	0	0	3
POSITION -4	0	1	0	1	0	1	1	1	0	3	2	0	1	2	0	0	1	0	2	0
POSITION -5	3	0	0	0	1	0	0	1	1	1	2	0	1	3	0	0	1	0	0	0
POSITION -6	2	0	0	0	0	0	2	0	0	1	1	1	1	1	0	1	0	0	0	1
POSITION -7	1	1	0	0	0	1	0	1	0	1	3	0	0	0	1	2	0	0	0	0
POSITION -8	2	0	0	0	0	0	0	0	0	0	3	2	1	0	0	0	0	2	0	0
POSITION -9	1	0	0	1	0	0	0	1	0	0	1	2	0	0	1	0	0	0	1	2
POSITION -10	0	1	0	1	0	0	1	1	0	0	0	0	2	0	0	1	1	1	0	1
POSITION -11	0	0	0	1	0	0	1	2	0	0	1	1	0	1	0	0	0	0	1	1
POSITION -12	2	0	0	0	0	1	0	0	0	0	2	0	0	0	0	1	0	0	1	0

Table 116: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of α -helices with crossing angles between -120° and -90° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	1	0	0	0	0	0	0	0	0	1	2	0	0	0	0	0	0	0	0	0
POSITION 11	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	4
POSITION 10	0	0	1	0	0	0	0	0	0	0	1	2	0	0	0	0	2	0	0	0
POSITION 9	0	1	0	0	0	0	3	0	0	0	0	0	0	0	1	2	1	0	0	0
POSITION 8	1	0	0	1	0	0	0	0	0	1	0	0	0	0	1	0	0	0	2	3
POSITION 7	2	0	0	0	1	0	0	1	0	0	2	1	0	1	0	2	0	0	0	0
POSITION 6	5	0	1	0	0	0	0	1	0	0	1	2	0	0	0	0	1	0	0	0
POSITION 5	0	0	0	0	1	1	0	0	0	0	4	4	0	0	0	0	1	0	1	1
POSITION 4	0	1	0	0	0	0	0	0	0	1	0	0	0	0	4	1	0	2	2	3
POSITION 3	2	0	2	0	0	0	0	0	1	1	3	4	0	0	1	1	0	0	0	1
POSITION 2	3	0	0	2	0	0	1	1	0	2	1	2	0	0	0	0	2	0	0	2
POSITION 1	1	0	0	1	0	0	0	5	0	0	4	3	0	1	0	0	0	0	0	1
POSITION 0	0	0	1	3	2	0	2	1	0	0	2	0	0	0	0	2	1	0	0	0
POSITION -1	8	0	0	1	0	1	0	1	0	0	0	1	0	0	0	1	0	0	0	2
POSITION -2	4	1	0	1	0	0	0	1	2	2	0	1	0	2	0	0	0	0	0	0
POSITION -3	1	1	0	0	0	0	0	5	0	0	1	0	0	1	0	0	0	0	0	2
POSITION -4	3	0	0	2	0	1	0	0	0	0	1	0	0	0	1	0	0	0	0	1
POSITION -5	0	1	0	1	0	0	0	1	0	0	0	0	0	3	0	0	0	0	1	0
POSITION -6	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	1	0	0	0
POSITION -7	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	2	0	0	0	1	0	0	0	0	0
POSITION -9	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -11	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
POSITION -12	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0

Table 117: Amino acid preferences by relative position with respect to nearest backbone contacts (display in yellow) with crossing angles between -150° and -137° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0
POSITION 11	0	1	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0
POSITION 10	1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0
POSITION 9	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0
POSITION 8	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	1	1	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	1	1	0	0	0	2	0	0	1	0	0
POSITION 6	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	3
POSITION 5	0	1	0	0	0	0	0	0	0	0	0	2	0	1	0	0	0	1	0	0
POSITION 4	1	0	0	0	0	1	1	0	0	0	1	1	1	0	0	0	0	1	0	0
POSITION 3	2	0	0	0	0	1	0	0	0	0	1	0	1	0	1	0	0	0	1	0
POSITION 2	0	1	0	1	0	0	0	2	0	0	1	1	0	0	0	1	0	0	0	0
POSITION 1	0	0	1	1	0	0	0	1	0	0	0	2	0	0	0	0	1	0	0	1
POSITION 0	1	0	0	0	0	0	1	0	0	0	3	0	0	0	0	0	0	0	1	1
POSITION -1	1	0	1	0	0	0	0	1	0	0	1	0	0	0	1	0	1	2	0	0
POSITION -2	1	0	0	0	0	1	1	1	1	0	1	1	0	0	0	0	0	1	0	0
POSITION -3	0	0	1	1	0	0	0	0	0	0	1	0	0	0	2	0	1	0	1	0
POSITION -4	1	0	0	0	0	1	0	0	1	1	1	0	0	0	0	0	0	0	0	0
POSITION -5	0	1	0	2	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0
POSITION -6	1	0	0	0	0	0	0	0	0	1	0	0	1	0	0	1	1	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0
POSITION -8	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0
POSITION -12	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

Table 118: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of α -helices with crossing angles between -180° and -150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	4	0	0	0	0	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	2	0	0	0	0	0	1	1	2	0	1	0	1	0	1	0	0	0	0
POSITION 10	0	0	1	1	0	2	0	1	1	1	1	0	1	0	2	1	0	0	0	0
POSITION 9	0	0	1	2	0	0	0	1	0	0	3	1	1	0	1	0	1	1	0	1
POSITION 8	1	0	0	1	0	1	1	0	0	0	1	0	1	0	1	2	1	0	0	3
POSITION 7	4	1	1	0	0	0	0	0	2	0	2	0	2	0	1	0	0	1	0	0
POSITION 6	3	0	1	0	0	0	0	2	0	0	5	1	0	0	0	1	0	0	1	1
POSITION 5	1	2	2	1	0	1	2	2	0	1	1	1	0	0	0	1	0	0	2	1
POSITION 4	1	0	1	0	0	0	1	1	1	1	4	4	2	0	0	0	3	2	0	0
POSITION 3	3	0	2	0	1	0	0	0	1	1	4	3	2	0	1	0	0	1	0	3
POSITION 2	4	2	0	0	1	2	0	2	1	0	1	1	1	0	0	0	2	2	0	3
POSITION 1	6	4	1	1	0	1	0	2	0	3	5	0	0	0	0	0	2	2	0	0
POSITION 0	5	1	1	1	0	1	1	0	0	1	1	0	1	0	3	3	0	1	2	0
POSITION -1	1	1	4	3	0	1	0	3	0	1	4	1	0	0	1	0	1	2	0	1
POSITION -2	4	0	2	2	0	3	0	0	0	0	2	4	0	0	1	2	1	0	0	0
POSITION -3	1	0	0	0	0	1	1	0	1	1	8	0	0	0	1	1	1	1	1	1
POSITION -4	3	1	0	0	0	1	1	1	1	2	1	0	1	0	2	0	2	2	0	1
POSITION -5	2	2	1	2	0	0	1	1	0	0	2	2	0	2	0	0	1	0	0	1
POSITION -6	1	0	1	1	0	1	1	0	1	0	1	4	1	0	0	0	0	0	0	0
POSITION -7	2	0	1	0	0	0	0	1	1	1	0	0	0	0	3	1	1	0	0	0
POSITION -8	0	1	0	2	0	1	0	1	2	0	2	0	0	0	0	0	0	0	1	0
POSITION -9	3	0	1	1	0	0	1	1	0	0	0	1	0	0	0	0	1	0	0	1
POSITION -10	1	0	0	1	0	0	2	0	0	1	0	1	0	0	0	0	0	0	0	1
POSITION -11	0	0	0	1	0	0	0	0	1	1	2	0	0	0	0	0	1	0	0	1
POSITION -12	1	0	0	0	1	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0

Table 119: Amino acid preferences by relative position with respect to nearest backbone contacts for α -helices and β -sheets with crossing angles between 0° and 30° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 1	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
POSITION -1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0
POSITION -2	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0
POSITION -4	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 120: Amino acid preferences by relative position with respect to nearest backbone contacts for α -helices and β -sheets with crossing angles between 30° and 60° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 121: Amino acid preferences by relative position with respect to nearest backbone contacts for α -helices and β -sheets with crossing angles between 60° and 90° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	1	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0
POSITION 10	1	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	1	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0
POSITION 7	0	0	0	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	1	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	1	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	1
POSITION 4	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	1
POSITION 3	0	0	0	0	0	0	1	2	0	0	0	0	0	0	0	2	0	0	0	0
POSITION 2	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	1	0	0	0
POSITION 1	0	0	0	0	1	0	0	0	0	0	0	1	0	0	2	0	0	1	0	0
POSITION 0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	1
POSITION -1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2	0	0	1
POSITION -2	1	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -3	0	0	0	1	0	0	0	0	1	0	0	0	0	0	1	0	1	0	0	0
POSITION -4	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1
POSITION -5	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0
POSITION -7	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -9	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0

Table 122: Amino acid preferences by relative position with respect to nearest backbone contacts for α -helices and β -sheets with crossing angles between 90° and 120° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	1	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	1	0	0	0	0
POSITION 9	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 7	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0
POSITION 6	0	0	0	1	0	0	0	2	0	0	0	0	0	0	1	0	0	0	0	0
POSITION 5	2	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
POSITION 4	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	2
POSITION 3	1	1	0	0	1	0	0	0	2	1	0	0	0	0	0	0	0	0	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	1	0	0	0	2	0	1	0	0	1	1
POSITION 1	1	0	0	0	0	0	0	0	0	1	0	1	0	0	0	2	0	0	0	0
POSITION 0	1	0	0	0	0	1	0	1	0	0	0	0	1	0	0	0	1	0	0	0
POSITION -1	0	0	0	0	0	0	0	0	0	0	0	0	2	0	1	1	0	0	0	1
POSITION -2	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	0	1	0	0
POSITION -3	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 123: Amino acid preferences by relative position with respect to nearest backbone contacts for α -helices and β -sheets with crossing angles between 120° and 150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	1	0	0	0	0	0	1	0	0	1	0	2	0	0	0	0	0	0	0	0
POSITION 11	1	0	0	1	0	0	0	0	0	1	2	0	0	0	0	0	0	0	0	0
POSITION 10	3	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	1	0	0	0
POSITION 9	0	0	0	1	0	1	2	1	0	0	0	2	0	0	0	0	0	0	0	0
POSITION 8	2	0	1	1	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	1
POSITION 7	1	0	0	0	0	0	0	0	0	2	0	0	0	0	1	1	0	0	1	2
POSITION 6	2	0	0	0	0	1	1	2	1	0	1	1	0	0	1	0	0	0	0	0
POSITION 5	0	0	1	3	0	1	1	0	0	0	0	0	1	1	0	0	1	1	0	1
POSITION 4	5	0	0	0	0	1	0	0	0	0	1	1	1	0	0	1	1	0	0	1
POSITION 3	2	1	0	1	0	0	1	0	0	2	0	1	3	0	0	0	0	0	0	1
POSITION 2	1	2	0	1	0	2	1	0	0	0	1	2	1	0	0	1	0	0	0	0
POSITION 1	2	1	1	1	0	0	1	0	0	2	0	1	0	0	0	1	1	1	0	0
POSITION 0	3	0	0	0	0	0	0	0	0	2	1	2	0	0	0	0	2	0	0	0
POSITION -1	2	0	1	0	0	2	0	0	0	0	1	0	2	0	0	0	1	0	0	1
POSITION -2	1	1	1	1	0	0	0	1	0	0	0	1	0	0	0	0	0	1	0	1
POSITION -3	0	0	0	0	0	0	2	0	0	1	0	0	0	1	1	0	1	0	0	1
POSITION -4	1	0	1	0	0	0	1	0	0	0	0	0	1	0	0	0	0	1	0	0
POSITION -5	0	0	0	0	0	0	1	1	0	0	0	0	0	0	1	0	0	0	0	1
POSITION -6	0	0	0	1	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0
POSITION -7	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0
POSITION -8	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 124: Amino acid preferences by relative position with respect to nearest backbone contacts for α -helices and β -sheets with crossing angles between 150° and 180° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	2	0	2	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	1
POSITION 11	2	1	0	0	0	0	0	0	0	1	1	1	0	0	0	0	1	0	0	1
POSITION 10	2	0	0	1	0	0	2	1	1	0	2	1	1	0	0	0	1	1	0	1
POSITION 9	0	1	0	0	0	2	2	3	0	0	1	5	0	0	0	1	0	1	0	0
POSITION 8	5	0	0	1	0	1	1	2	0	1	1	0	1	0	0	3	0	0	0	1
POSITION 7	0	0	0	0	0	0	2	0	0	3	3	0	0	0	0	0	0	2	1	6
POSITION 6	0	1	0	0	0	0	0	1	2	3	1	1	0	0	2	0	2	2	1	1
POSITION 5	3	0	1	2	0	0	1	1	1	0	2	1	0	2	0	1	1	1	0	1
POSITION 4	8	2	0	0	0	0	0	1	0	1	1	1	0	0	0	1	2	0	0	2
POSITION 3	6	2	0	1	1	0	1	0	0	1	1	0	2	0	1	0	0	0	1	1
POSITION 2	3	1	2	0	0	1	2	0	1	0	2	2	2	0	0	0	0	1	1	1
POSITION 1	3	0	0	0	0	0	5	3	0	0	0	2	0	0	0	2	2	2	0	0
POSITION 0	4	0	0	0	0	1	0	1	2	0	1	0	0	1	0	0	3	0	0	2
POSITION -1	3	2	1	1	0	0	1	0	3	0	1	0	1	0	0	0	0	1	0	2
POSITION -2	0	0	1	3	0	0	3	0	2	0	1	1	0	1	1	1	0	0	0	0
POSITION -3	0	0	1	0	0	1	0	1	1	0	0	0	0	2	1	1	1	1	0	2
POSITION -4	2	0	0	0	0	0	0	0	0	2	0	0	0	0	1	3	1	0	0	1
POSITION -5	4	0	0	0	0	1	0	0	0	0	0	2	0	1	0	0	0	1	0	0
POSITION -6	1	0	0	0	0	1	3	0	0	0	0	1	1	0	0	0	1	1	0	0
POSITION -7	2	1	0	2	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	1
POSITION -8	1	0	0	0	0	1	1	0	1	0	0	0	0	0	0	0	0	1	1	0
POSITION -9	0	0	1	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -10	1	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
POSITION -12	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 125: Amino acid preferences by relative position with respect to nearest backbone contacts for α -helices and β -sheets with crossing angles between -30° and 0° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION 10	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0
POSITION 6	2	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	1	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1
POSITION 3	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0
POSITION 2	0	0	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	1
POSITION 0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1
POSITION -1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0
POSITION -2	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
POSITION -3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -5	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 126: Amino acid preferences by relative position with respect to nearest backbone contacts for α -helices and β -sheets with crossing angles between -60° and -30° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1
POSITION 6	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
POSITION 5	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 3	1	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0
POSITION 2	0	0	1	0	0	0	0	0	0	0	1	0	1	0	0	0	1	0	0	0
POSITION 1	0	0	0	0	0	0	1	0	0	1	0	1	0	0	0	1	0	0	0	0
POSITION 0	1	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -1	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	0	0	0
POSITION -2	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
POSITION -3	0	0	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	1	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0
POSITION -6	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -9	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 127: Amino acid preferences by relative position with respect to nearest backbone contacts for α -helices and β -sheets with crossing angles between -90° and -60° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 128: Amino acid preferences by relative position with respect to nearest backbone contacts for α -helices and β -sheets with crossing angles between -120° and -90° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
POSITION 2	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
POSITION 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
POSITION -1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION -2	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION -3	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 129: Amino acid preferences by relative position with respect to nearest backbone contacts for α -helices and β -sheets with crossing angles between -150° and -120° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0
POSITION 1	0	1	0	0	0	1	1	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -1	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0
POSITION -2	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0
POSITION -3	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0
POSITION -6	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0
POSITION -7	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
POSITION -10	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

Table 130: Amino acid preferences by relative position with respect to nearest backbone contacts for α -helices and β -sheets with crossing angles between -180° and -150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 11	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	1	0	0	0
POSITION 5	1	0	0	0	1	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 4	0	1	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0
POSITION 3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2	0	1	0	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1	1	0	0
POSITION 1	0	0	0	0	0	1	1	0	1	1	0	0	0	0	0	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	2	0	0	0	0	0
POSITION -1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
POSITION -2	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -3	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 131: Amino acid preferences by relative position with respect to nearest backbone contacts for β -sheets and α -helices with crossing angles between 0° and 30° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
POSITION 4	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -2	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0
POSITION -3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 132: Amino acid preferences by relative position with respect to nearest backbone contacts for β -sheets and α -helices with crossing angles between 30° and 60° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 133: Amino acid preferences by relative position with respect to nearest backbone contacts for β -sheets and α -helices with crossing angles between 60° and 90° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0
POSITION 3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
POSITION 2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0
POSITION 1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 0	0	0	1	0	0	0	0	1	0	1	0	0	0	0	0	0	1	0	0	0
POSITION -1	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0
POSITION -2	0	0	0	0	0	1	0	0	0	0	1	1	0	0	0	0	0	0	0	1
POSITION -3	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 134: Amino acid preferences by relative position with respect to nearest backbone contacts for β -sheets and α -helices with crossing angles between 90° and 120° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1
POSITION 5	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0
POSITION 3	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1
POSITION 1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	1
POSITION 0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	1
POSITION -1	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	1
POSITION -2	0	0	0	0	0	0	0	0	0	0	0	1	2	0	0	1	0	1	0	0
POSITION -3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2
POSITION -4	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 135: Amino acid preferences by relative position with respect to nearest backbone contacts for β -sheets and α -helices with crossing angles between 120° and 150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 7	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0
POSITION 3	1	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	1
POSITION 1	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	1	1	0	0	1
POSITION 0	1	0	0	0	0	1	0	0	0	3	3	0	0	0	0	1	0	0	0	0
POSITION -1	2	0	1	0	0	0	0	4	0	0	1	0	0	0	1	0	1	0	0	0
POSITION -2	0	0	0	0	0	0	1	0	0	2	1	0	1	0	2	0	0	0	0	3
POSITION -3	1	0	0	0	0	0	0	0	0	2	1	0	0	0	1	0	1	0	0	2
POSITION -4	2	0	0	0	0	1	0	0	0	0	1	1	0	0	0	0	0	0	0	1
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 136: Amino acid preferences by relative position with respect to nearest backbone contacts for β -sheets and α -helices with crossing angles between 150° and 180° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	1	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	1	0	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	1	0	1	0	0	1	0	0	1	0	3
POSITION 1	1	0	0	0	0	1	0	1	1	0	2	0	0	0	2	1	0	1	0	2
POSITION 0	2	0	2	0	0	0	0	1	0	3	1	0	0	0	0	0	1	0	0	3
POSITION -1	1	1	0	2	0	0	0	1	0	2	1	0	0	1	2	3	0	0	0	4
POSITION -2	1	0	0	0	0	0	0	1	0	3	2	0	0	0	1	1	1	0	0	4
POSITION -3	0	2	0	0	0	0	0	0	0	2	0	1	0	1	2	0	0	0	0	4
POSITION -4	0	0	0	0	0	0	0	1	0	1	2	0	0	0	1	0	0	1	0	0
POSITION -5	1	0	0	0	0	1	1	0	0	0	1	0	0	0	0	0	0	0	0	1
POSITION -6	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	2
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 137: Amino acid preferences by relative position with respect to nearest backbone contacts for β -sheets and α -helices with crossing angles between -30° and 0° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	1
POSITION 1	0	0	0	2	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0
POSITION -2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION -3	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 138: Amino acid preferences by relative position with respect to nearest backbone contacts for β -sheets and α -helices with crossing angles between -60° and -30° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
POSITION 4	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
POSITION 3	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0
POSITION 1	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION -1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION -2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
POSITION -3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 139: Amino acid preferences by relative position with respect to nearest backbone contacts for β -sheets and α -helices with crossing angles between -90° and -60° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 140: Amino acid preferences by relative position with respect to nearest backbone contacts for β -sheets and α -helices with crossing angles between -120° and -90° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
POSITION -1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
POSITION -2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 141: Amino acid preferences by relative position with respect to nearest backbone contacts for β -sheets and α -helices with crossing angles between -150° and -120° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0
POSITION 2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 1	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	1
POSITION 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -1	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION -2	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0
POSITION -3	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0
POSITION -5	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 142: Amino acid preferences by relative position with respect to nearest backbone contacts for β -sheets and α -helices with crossing angles between -180° and -150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0
POSITION 2	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0
POSITION 1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
POSITION -1	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -2	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0
POSITION -3	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 143: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of β -sheets with crossing angles between 0° and 30° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
POSITION 1	1	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	2	0	0	0
POSITION 0	0	0	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	1
POSITION -1	0	0	1	0	0	0	0	1	0	0	2	0	0	1	1	1	0	0	0	0
POSITION -2	0	0	0	0	0	1	0	0	0	1	1	1	0	0	0	1	0	0	0	2
POSITION -3	0	2	0	1	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	1
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	2
POSITION -5	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 144: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of β -sheets with crossing angles between 30° and 60° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -1	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -2	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0
POSITION -3	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
POSITION -5	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 145: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of β -sheets with crossing angles between 60° and 90° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
POSITION 2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 1	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0
POSITION 0	0	1	0	0	1	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0
POSITION -1	0	0	0	0	0	1	0	0	0	0	1	0	0	0	1	0	0	0	0	0
POSITION -2	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0
POSITION -3	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
POSITION -4	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
POSITION -7	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 146: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of β -sheets with crossing angles between 90° and 120° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
POSITION 7	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
POSITION 6	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0
POSITION 5	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	2
POSITION 3	2	0	0	0	0	0	0	0	0	0	0	1	1	0	2	1	1	0	0	0
POSITION 2	1	1	0	0	0	1	0	0	0	2	1	1	0	0	1	3	1	0	0	2
POSITION 1	0	1	0	0	0	0	0	0	1	3	1	4	1	0	2	1	0	0	0	3
POSITION 0	3	1	0	0	0	0	1	2	0	1	2	1	1	0	1	2	1	1	1	1
POSITION -1	0	0	0	0	0	0	0	2	0	1	5	2	0	0	1	2	2	1	0	5
POSITION -2	2	0	0	2	1	2	1	0	0	1	0	3	0	0	1	0	1	0	0	2
POSITION -3	1	0	0	0	1	0	0	0	0	2	4	1	0	1	0	0	1	0	1	1
POSITION -4	0	0	1	0	0	0	0	0	0	1	1	1	0	2	1	0	1	0	0	2
POSITION -5	0	0	0	0	0	1	1	0	0	0	2	1	0	0	0	0	1	0	1	0
POSITION -6	0	0	0	0	0	0	0	0	0	1	2	0	0	0	0	2	0	1	0	0
POSITION -7	0	0	0	1	0	0	0	0	0	0	1	1	0	0	0	0	1	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0
POSITION -9	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 147: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of β -sheets with crossing angles between 120° and 150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	1	0	0	0	0	1	1	0	1	0	0	0	0	0	0	0	0	1	0	1
POSITION 7	1	0	0	0	0	0	1	2	0	1	0	0	1	0	1	0	0	0	0	0
POSITION 6	1	0	1	0	0	0	0	1	2	0	0	1	0	0	1	1	0	1	0	1
POSITION 5	2	1	1	0	1	2	0	1	3	3	0	0	1	0	1	1	1	1	1	1
POSITION 4	3	0	1	2	0	1	1	1	0	1	3	0	0	0	4	2	3	1	1	4
POSITION 3	1	0	1	0	1	2	4	3	2	2	0	2	1	2	4	1	3	2	0	8
POSITION 2	4	0	1	1	1	1	3	1	1	5	3	3	3	1	5	6	4	1	0	4
POSITION 1	5	1	1	1	2	2	1	1	2	4	8	2	5	2	3	2	6	2	4	5
POSITION 0	3	4	0	0	0	2	1	3	2	6	4	4	1	0	6	4	7	4	1	5
POSITION -1	5	1	2	2	0	0	2	3	2	3	8	2	0	0	7	4	6	3	0	10
POSITION -2	7	3	3	2	1	1	3	0	0	1	3	0	0	0	4	5	4	3	0	9
POSITION -3	0	1	2	1	1	1	0	6	1	4	4	1	1	0	0	2	2	2	0	10
POSITION -4	3	0	0	0	0	0	2	1	2	1	3	0	3	3	2	1	0	2	0	3
POSITION -5	0	1	0	1	0	0	1	3	0	2	1	2	2	0	3	2	1	2	0	0
POSITION -6	1	1	0	1	1	0	2	1	0	1	0	0	1	0	0	1	1	0	1	1
POSITION -7	2	1	0	0	0	0	0	0	1	0	0	0	0	0	1	1	1	0	0	1
POSITION -8	1	0	0	0	1	0	0	1	0	1	0	1	0	0	0	0	0	0	0	0
POSITION -9	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
POSITION -10	1	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 148: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of β -sheets with crossing angles between 150° and 180° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	1	0	0	0	0
POSITION 7	0	0	0	0	0	1	1	1	0	0	1	2	0	0	1	0	0	0	0	1
POSITION 6	2	0	0	0	0	0	1	0	0	0	3	0	0	1	0	2	1	0	0	2
POSITION 5	2	2	1	0	0	0	1	1	0	2	5	3	1	0	3	1	3	0	0	1
POSITION 4	3	1	0	0	0	1	1	1	0	4	5	0	1	2	3	1	1	1	0	10
POSITION 3	5	2	1	1	2	0	3	4	1	2	3	3	0	1	2	3	6	4	2	4
POSITION 2	2	1	1	2	5	2	1	3	1	5	9	4	1	2	3	3	4	2	2	7
POSITION 1	6	0	2	5	2	4	3	2	1	2	9	5	0	1	1	12	4	5	1	10
POSITION 0	6	1	3	0	1	1	4	4	1	8	5	1	3	0	7	3	5	9	0	6
POSITION -1	4	1	2	2	2	2	5	1	1	5	11	2	3	2	3	6	6	4	2	9
POSITION -2	6	2	1	2	2	5	1	2	0	6	7	2	1	0	4	3	1	3	1	9
POSITION -3	1	3	0	2	2	0	2	2	2	3	7	3	1	2	0	3	4	2	1	8
POSITION -4	2	1	1	2	0	2	0	0	1	4	2	1	0	1	0	2	4	1	0	4
POSITION -5	3	1	1	1	1	3	2	0	0	0	1	1	0	2	3	1	1	1	0	0
POSITION -6	0	0	0	0	0	1	0	0	0	3	1	2	1	0	0	0	0	0	0	2
POSITION -7	1	0	0	0	0	1	1	0	0	0	1	0	0	0	0	0	1	0	0	1
POSITION -8	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1
POSITION -9	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
POSITION -11	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0

Table 149: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of β -sheets with crossing angles between -30° and 0° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3
POSITION 4	1	0	0	0	0	0	0	0	0	2	2	1	1	0	1	0	1	0	0	4
POSITION 3	1	0	2	0	0	0	0	1	0	2	3	3	1	1	0	0	0	1	0	5
POSITION 2	3	0	0	0	1	0	0	0	0	6	4	1	1	0	3	3	1	1	0	5
POSITION 1	5	2	0	0	0	0	0	3	1	4	1	2	2	1	4	1	2	2	0	10
POSITION 0	1	0	1	1	0	2	1	5	0	7	6	0	1	0	3	0	0	2	0	8
POSITION -1	5	2	1	0	0	1	1	2	0	8	6	1	1	0	4	1	0	0	3	7
POSITION -2	2	0	0	0	0	0	1	0	0	6	7	2	0	1	0	0	4	1	1	7
POSITION -3	1	1	1	0	0	0	0	0	0	3	3	2	1	0	0	1	0	2	0	5
POSITION -4	0	1	0	0	1	0	0	1	0	0	2	1	0	0	1	0	1	0	0	3
POSITION -5	0	0	0	0	1	0	0	0	0	0	3	0	0	0	1	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 150: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of β -sheets with crossing angles between -60° and -30° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
POSITION 7	0	0	0	0	0	0	0	0	0	1	1	0	1	0	0	1	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	1	0	0	2	0	0	0	0	0	0	0	0	1
POSITION 5	0	0	0	1	0	0	0	0	0	0	2	0	0	1	1	1	0	0	0	1
POSITION 4	0	0	0	0	0	0	0	2	1	0	3	1	0	0	0	0	1	0	0	0
POSITION 3	1	0	0	1	0	1	1	0	0	2	1	0	0	0	0	0	0	0	0	2
POSITION 2	0	0	0	0	0	0	0	0	1	1	1	0	0	0	3	1	2	0	0	3
POSITION 1	2	0	0	0	0	2	0	0	0	1	2	1	0	0	3	1	0	0	1	4
POSITION 0	1	0	0	0	0	1	1	0	0	3	1	0	1	0	0	1	1	0	0	3
POSITION -1	1	0	0	0	0	0	1	1	0	2	0	0	0	1	0	1	1	0	0	6
POSITION -2	1	1	1	0	1	0	0	0	0	1	1	0	0	0	0	0	0	0	0	2
POSITION -3	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
POSITION -4	1	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 151: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of β -sheets with crossing angles between -90° and -60° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 3	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 2	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
POSITION 1	0	0	0	0	0	0	0	0	0	2	2	0	0	0	0	0	0	0	0	0
POSITION 0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	2	0
POSITION -1	0	0	0	0	0	0	0	0	1	2	2	0	0	0	0	1	0	0	0	0
POSITION -2	0	0	0	0	0	2	0	1	0	0	1	0	0	0	0	0	1	0	0	0
POSITION -3	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION -4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 152: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of β -sheets with crossing angles between -120° and -90° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
POSITION 6	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1
POSITION 3	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0
POSITION 2	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	2	0	0	0
POSITION 1	0	0	0	0	0	0	0	0	0	1	3	0	0	0	0	0	1	2	1	0
POSITION 0	1	0	0	0	0	0	0	0	0	0	3	0	0	0	1	1	0	0	0	0
POSITION -1	2	0	0	0	0	0	0	0	0	2	0	2	0	0	0	1	0	1	0	2
POSITION -2	1	0	0	0	1	0	0	0	1	0	0	0	0	1	0	0	2	2	0	0
POSITION -3	0	0	0	0	0	0	0	0	0	4	0	0	0	1	0	0	0	0	0	2
POSITION -4	1	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	2	0	0
POSITION -5	1	0	0	0	0	0	0	0	0	0	2	0	0	1	0	0	0	0	0	2
POSITION -6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	2	0	0	0	1
POSITION -7	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -8	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0
POSITION -9	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 153: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of β -sheets with crossing angles between -150° and -120° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	0	0	0	1	0	0	0	0	0	2	0	0	0	0	1	0	1	0	0	0
POSITION 3	0	0	0	1	0	0	0	0	1	1	2	0	0	0	0	0	1	0	0	0
POSITION 2	0	1	0	0	0	0	0	1	0	2	0	0	0	0	1	0	0	0	1	0
POSITION 1	0	0	0	0	0	2	0	0	0	0	0	0	0	0	1	1	1	0	0	1
POSITION 0	0	1	0	0	0	0	0	0	0	2	1	0	0	0	2	0	0	0	0	1
POSITION -1	0	0	2	0	0	0	0	0	0	0	3	0	0	1	0	0	0	0	0	2
POSITION -2	1	1	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	1	0	2
POSITION -3	0	0	0	0	0	1	0	0	1	0	2	0	0	0	0	0	1	1	0	0
POSITION -4	0	0	0	0	0	0	1	0	1	0	0	0	0	0	1	0	1	0	1	0
POSITION -5	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	1	0	0	0
POSITION -6	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	1	0	0	0
POSITION -7	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0
POSITION -8	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -9	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION -11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 154: Amino acid preferences by relative position with respect to nearest backbone contacts for pairs of β -sheets with crossing angles between -180° and -150° .

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1
POSITION 9	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	1	0	0	0	0
POSITION 8	1	0	2	0	0	0	0	1	0	0	2	0	0	1	0	0	0	0	0	0
POSITION 7	0	0	0	0	0	0	1	0	0	1	1	0	1	0	0	1	1	2	0	0
POSITION 6	2	0	0	0	0	0	0	1	0	1	2	0	0	0	4	0	1	0	0	1
POSITION 5	1	1	0	0	0	2	1	2	0	0	1	2	1	0	0	1	0	2	0	2
POSITION 4	0	3	1	1	2	0	0	1	0	2	1	0	1	0	1	0	1	1	0	2
POSITION 3	2	1	0	0	0	0	1	2	0	3	1	1	0	0	1	2	1	1	1	1
POSITION 2	0	0	0	0	0	0	0	1	3	5	1	2	0	0	0	4	2	2	0	3
POSITION 1	4	3	0	0	0	2	1	2	0	1	3	1	0	2	0	1	2	0	0	2
POSITION 0	0	1	0	2	0	1	0	0	1	1	3	0	0	0	4	1	2	0	1	3
POSITION -1	4	2	0	0	0	1	1	0	0	1	2	1	0	0	2	1	3	3	0	5
POSITION -2	2	1	0	0	0	0	1	0	1	1	2	0	1	2	0	3	3	1	1	3
POSITION -3	0	2	0	1	0	0	0	1	0	0	0	1	0	0	3	0	2	4	2	2
POSITION -4	0	0	1	0	0	0	0	2	3	1	2	0	0	0	0	1	4	0	0	2
POSITION -5	1	0	0	1	0	2	0	1	1	0	2	0	0	0	0	3	1	2	1	0
POSITION -6	1	0	0	1	2	0	0	1	0	1	1	0	0	0	1	1	0	0	0	1
POSITION -7	0	0	1	0	0	0	0	2	0	0	2	1	0	1	1	0	0	0	0	0
POSITION -8	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0
POSITION -9	1	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0
POSITION -10	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0
POSITION -11	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION -12	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0

APPENDIX K

Table 155: Number of interactions between oppositely charged atoms and average number of atom contacts at each position for interactions between pairs of α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	1	0	1	0	2	0	3	0	0	0	0	1	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	4.0	0.0	4.0	0.0	2.5	0.0	2.7	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	2	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	1	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	1	1	1	3	1	1	0	3	1	1	0	3	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	2.0	4.0	2.0	4.0	2.0	0.0	1.3	2.0	3.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	1	1	2	0	0	2	1	0	0	1	0	1	0	1	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	2.0	1.0	0.0	0.0	1.5	2.0	0.0	0.0	1.0	0.0	3.0	0.0	2.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	1	0	0	0	0	0	1	1	1	0	0	1	0	0	0	1	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	2	2	0	0	0	1	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	0.0	0.0	4.0	0.0	0.0	3.0	3.0	0.0	0.0	0.0	4.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	1	0	1	0	0	0	1	0	2	1	0	0	1	0	1	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	3.0	0.0	3.0	0.0	0.0	0.0	2.0	0.0	1.5	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	1	0	0	1	4	0	2	4	0	0	2	2	0	0	1	1	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	1.0	2.2	0.0	3.0	2.5	0.0	0.0	2.0	1.5	0.0	0.0	3.0	1.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	2	0	0	2	0	0	2	0	0	1	1	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	2.0	0.0	0.0	2.0	0.0	0.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	2.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	3.0	0.0	0.0

Table 156: Number of interactions between oppositely charged atoms and average number of atom contacts at each position for interactions between α -helices and β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 157: Number of interactions between oppositely charged atoms and average number of atom contacts at each position for interactions between β -sheets and α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 158: Number of interactions between oppositely charged atoms and average number of atom contacts at each position for interactions between pairs of β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	1	0	0	0	0	2	0	0	1	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	1	0	1	0	5	2	1	1	0	1	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	2.0	0.0	1.2	2.0	2.0	2.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	1	0	2	0	1	0	2	0	2	1	1	0	1	0	1	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	2.0	0.0	3.0	0.0	2.0	0.0	1.0	0.0	1.5	1.0	2.0	0.0	4.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	1	0	0	1	1	0	0	0	1	0	0	0	0	0	1	2	0	0	0	1	0	0	0
-180	-150	0.0	0.0	3.0	0.0	0.0	1.0	2.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	2.0	1.5	0.0	0.0	3.0	0.0	0.0	0.0	0.0

Table 159: Number of interactions between atoms of like charge and average number of atom contacts at each position for interactions between pairs of α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	1	0	0	0	0	0	0	0	0	0	0	2	0	0	0	1	1	0	0	1	0	0	0	0
120	150	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	3.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	1	1	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	1.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	1	0	1	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	3.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 160: Number of interactions between atoms of like charge and average number of atom contacts at each position for interactions between α -helices and β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 161: Number of interactions between atoms of like charge and average number of atom contacts at each position for interactions between β -sheets and α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 162: Number of interactions between atoms of like charge and average number of atom contacts at each position for interactions between pairs of β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	0.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 163: Number of interactions between charged atoms and polar side-chain atoms and average number of atom contacts at each position for interactions between pairs of α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	1	0	0	1	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	1	0	2	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	2	0	1	1	1	0	3	0	0	0	2	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	1.5	0.0	1.0	1.0	1.0	0.0	1.3	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	2	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	1	0	0	2	0	2	0	1	1	0	1	1	0	0	2	0	0	1	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	1.0	2.0	0.0	3.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	2	0	1	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	1	2	2	0	2	0	0	0	0	0	0	0	1	0	0	0	0	0	1	1	0
-180	-150	0.0	0.0	0.0	0.0	1.0	1.0	1.5	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	0.0

Table 164: Number of interactions between charged atoms and polar side-chain atoms and average number of atom contacts at each position for interactions between α -helices and β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 165: Number of interactions between charged atoms and polar side-chain atoms and average number of atom contacts at each position for interactions between β -sheets and α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 166: Number of interactions between charged atoms and polar side-chain atoms and average number of atom contacts at each position for interactions between pairs of β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	1	0	0	1	0	2	1	0	1	0	1	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	2	1	2	1	2	4	0	0	0	0	1	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	2.0	1.0	1.0	1.5	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	1	3	1	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.3	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	1	0	1	1	0	0	0	0	0	1	1	0	1	0	0	1	0	0	0	0	0	0	0	0	0
-180	-150	1.0	0.0	1.0	2.0	0.0	0.0	0.0	0.0	0.0	1.0	2.0	0.0	2.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 167: Number of interactions between charged atoms and backbone oxygen atoms and average number of atom contacts at each position for interactions between pairs of α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	3	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	2	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	1	3	0	0	2	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
150	180	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	3	2	0	0	0	0	1	0	0	0	2	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	1	0	1	0	2	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	1	0	0	0	2	1	0	0	2	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	2.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 168: Number of interactions between charged atoms and backbone oxygen atoms and average number of atom contacts at each position for interactions between α -helices and β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	1	1	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0
150	180	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 169: Number of interactions between charged atoms and backbone oxygen atoms and average number of atom contacts at each position for interactions between pairs of β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	2	0	0	0	2	0	0	0	0	4	0	1	0	0	1	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	1	1	0	1	0	1	2	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	1	0	1	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 170: Number of interactions between charged atoms and backbone nitrogen atoms and average number of atom contacts at each position for interactions between pairs of α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 171: Number of interactions between charged atoms and backbone nitrogen atoms and average number of atom contacts at each position for interactions between pairs of β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	1	0	3	0	0	0	0	2	1	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 172: Number of interactions between polar side-chain atoms and average number of atom contacts at each position for interactions between pairs of α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	1	0	0	0	0	0	0	0	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
30	60	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	1	0	0	0	2	0	0	0	0	1	0	0	1	0	0	0	3	0	0	0	0
120	150	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
150	180	1	1	0	0	0	1	0	0	1	0	0	1	1	0	0	0	1	1	1	0	0	0	1	1	0
150	180	1.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	2.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	2.0	1.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	4	0	0	0	1	0	0	1	1	0	0	1	2	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	3	2	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	2	1	1	0	0	2	0	0	2	0	0	1	3	0	1	2	0	0	1	0	0
-180	-150	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0

Table 173: Number of interactions between polar side-chain atoms and average number of atom contacts at each position for interactions between α -helices and β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	2	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 174: Number of interactions between polar side-chain atoms and average number of atom contacts at each position for interactions between β -sheets and α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 175: Number of interactions between polar side-chain atoms and average number of atom contacts at each position for interactions between pairs of β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	1	1	0	0	0	2	0	0	0	1	0	0	1	0	0	1	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	2	3	2	2	1	2	2	0	2	1	1	1	1	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.5	1.0	1.0	1.0	1.5	0.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	1	8	1	6	2	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	1	4	1	0	2	1	1	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	1	0	1	0	2	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	1	0	0	0	0	0	2	0	1	0	1	0	1	0	1	0	0	0	0	2	0	0	0	1
-180	-150	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	1.0

Table 176: Number of interactions between polar side-chain atoms and backbone oxygen atoms and average number of atom contacts at each position for interactions between pairs of α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	2	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	2	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	3	2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	1	3	0	1	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	1	0	0	1	2	0	0	0	1	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 177: Number of interactions between polar side-chain atoms and backbone oxygen atoms and average number of atom contacts at each position for interactions between α -helices and β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	1	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 178: Number of interactions between polar side-chain atoms and backbone oxygen atoms and average number of atom contacts at each position for interactions between β -sheets and α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 179: Number of interactions between polar side-chain atoms and backbone oxygen atoms and average number of atom contacts at each position for interactions between pairs of β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	1	0	0	2	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	3	0	2	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	1	0	1	0	0	1	0	0	1	2	1	0	0	1	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	1	3	0	2	0	2	0	1	0	2	1	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	1.0	0.0	1.0	0.0	1.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	2	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	1	0	1	0	0	0	0	0	0	1	0	1	1	0	1	1	0	0	0	0	1
-180	-150	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	1.0

Table 180: Number of interactions between polar side-chain atoms and backbone nitrogen atoms and average number of atom contacts at each position for interactions between pairs of α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 181: Number of interactions between polar side-chain atoms and backbone nitrogen atoms and average number of atom contacts at each position for interactions between α -helices and β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 182: Number of interactions between polar side-chain atoms and backbone nitrogen atoms and average number of atom contacts at each position for interactions between β -sheets and α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 183: Number of interactions between polar side-chain atoms and backbone nitrogen atoms and average number of atom contacts at each position for interactions between pairs of β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	1	0	0	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	1	0	0	0	0	1	0	2	0	0	0	0	1	1	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 184: Number of interactions between backbone atoms and average number of atom contacts at each position for interactions between pairs of α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	3	3	0	0	6	2	0	4	9	1	0	1	1	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	1.7	2.3	0.0	0.0	1.7	2.0	0.0	1.0	2.0	1.0	0.0	2.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	3	2	0	3	10	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.7	1.0	0.0	2.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	1	0	0	0	2	0	0	1	1	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	1	0	0	1	7	3	0	5	19	5	0	3	9	5	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	2.0	0.0	0.0	1.0	1.4	2.3	0.0	1.6	2.5	1.6	0.0	1.0	2.0	1.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	2	0	0	1	1	0	2	14	13	0	3	34	10	0	4	11	3	1	1	2	0	0	1	0
120	150	0.0	1.5	0.0	0.0	1.0	1.0	0.0	1.0	1.6	1.5	0.0	1.0	1.4	1.9	0.0	1.2	1.7	1.0	3.0	1.0	1.0	0.0	0.0	1.0	0.0
150	180	0	1	0	1	1	1	0	1	3	1	0	5	20	3	0	3	8	0	0	3	1	0	0	1	0
150	180	0.0	5.0	0.0	3.0	1.0	1.0	0.0	1.0	1.3	1.0	0.0	1.2	1.4	1.3	0.0	2.0	2.0	0.0	0.0	1.7	2.0	0.0	0.0	3.0	0.0
-30	0	0	1	0	0	0	1	0	0	2	0	0	1	11	3	0	3	5	1	0	0	3	1	0	0	0
-30	0	0.0	1.0	0.0	0.0	0.0	3.0	0.0	0.0	1.5	0.0	0.0	2.0	1.6	1.0	0.0	1.7	1.8	3.0	0.0	0.0	1.7	2.0	0.0	0.0	0.0
-60	-30	0	0	0	0	5	2	0	3	21	13	0	9	33	8	0	4	15	4	0	1	2	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	1.0	1.0	0.0	1.3	1.6	1.8	0.0	1.6	1.7	1.2	0.0	1.2	1.9	1.5	0.0	4.0	1.5	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	6	2	0	3	10	1	0	1	2	0	0	0	1	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3	1.5	0.0	1.7	1.4	2.0	0.0	2.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	4	7	0	2	13	3	0	2	3	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.6	0.0	1.5	1.6	2.7	0.0	1.5	1.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	1	2	2	3	1	0	2	2	0	0	0	1	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.5	1.5	2.0	2.0	0.0	1.0	1.5	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
-180	-150	0	0	1	0	2	3	0	0	8	5	0	3	13	3	0	7	9	0	0	5	0	0	1	1	0
-180	-150	0.0	0.0	2.0	0.0	1.0	1.3	0.0	0.0	1.6	1.4	0.0	1.0	2.0	1.0	0.0	1.6	2.2	0.0	0.0	2.0	0.0	0.0	1.0	2.0	0.0

Table 185: Number of interactions between backbone atoms and average number of atom contacts at each position for interactions between α -helices and β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	2	1	0	0	1	1	0	1	1	0	1	1	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.5	1.0	0.0	0.0	1.0	2.0	0.0	1.0	1.0	0.0	1.0	3.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	1	4	0	0	0	1	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.8	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	1	0	0	0	0	0	0	0	0	0	1	5	0	0	1	3	0	0	0	0	0	0	0	0
120	150	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	1.4	0.0	0.0	1.0	1.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	1	1	0	1	3	2	0	2	11	3	0	2	7	1	0	2	3	0	0	0	0
150	180	0.0	0.0	0.0	0.0	1.0	2.0	0.0	2.0	2.3	1.5	0.0	1.5	1.8	1.7	0.0	1.0	1.4	3.0	0.0	1.5	2.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	3	1	0	0	2	0	0	0	0	0	1	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	4.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
-60	-30	0	1	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 186: Number of interactions between backbone atoms and average number of atom contacts at each position for interactions between β -sheets and α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	1	1	2	6	4	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	1.8	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	1	2	3	5	1	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.0	2.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	1	6	7	1	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.5	1.1	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	1	1	8	6	5	3	1	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	4.0	1.7	1.7	1.6	1.3	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	1	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 187: Number of interactions between backbone atoms and average number of atom contacts at each position for interactions between pairs of β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	1	0	4	2	3	2	4	1	2	0	1	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	4.7	1.5	2.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	1	0	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	2.0	5.0	1.0	1.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	1	2	0	1	4	2	2	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.5	0.0	1.0	1.8	2.5	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	1	0	1	2	6	3	13	8	25	9	10	7	2	0	1	1	0	1	0	0	0
90	120	0.0	0.0	0.0	0.0	1.0	0.0	1.0	1.5	1.2	1.7	1.8	2.2	1.9	1.9	1.3	2.0	1.0	0.0	3.0	2.0	0.0	1.0	0.0	0.0	0.0
120	150	0	0	1	1	1	3	7	6	24	11	40	13	59	24	26	7	11	6	3	1	6	1	0	0	0
120	150	0.0	0.0	2.0	2.0	2.0	1.0	1.7	1.2	1.6	1.8	1.3	1.6	1.6	1.5	1.4	1.0	1.7	1.8	2.0	1.0	1.7	1.0	0.0	0.0	0.0
150	180	0	1	0	0	1	3	15	10	26	8	39	9	67	29	34	11	16	8	5	3	1	0	0	0	0
150	180	0.0	2.0	0.0	0.0	1.0	1.3	1.6	1.3	1.7	1.2	1.2	1.6	1.4	1.2	1.2	1.5	1.4	1.2	1.0	2.3	1.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	4	3	11	4	17	6	32	14	16	10	8	1	2	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.3	1.3	1.2	1.2	1.8	1.8	2.1	1.4	1.2	1.1	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	1	2	1	7	2	5	4	8	1	1	1	4	0	2	1	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.5	1.0	1.0	1.0	3.2	1.8	1.4	2.0	1.0	2.0	1.0	0.0	2.5	3.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	2	0	3	4	6	1	1	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	1.7	1.2	1.7	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	2	3	4	2	8	3	9	3	5	1	0	2	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	1.5	1.3	1.8	2.5	1.5	1.3	2.0	1.7	1.4	2.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	1	1	3	0	1	0	7	1	8	4	4	0	4	1	2	1	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	1.0	2.0	1.0	0.0	1.0	0.0	1.3	1.0	1.2	1.2	1.2	0.0	1.2	1.0	1.5	1.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	1	0	1	3	5	7	6	10	3	13	7	30	12	21	7	13	7	7	4	3	0	1	0	0
-180	-150	0.0	1.0	0.0	1.0	1.3	2.2	1.7	2.2	1.7	1.0	1.4	1.0	1.3	1.5	1.8	1.3	1.4	1.7	1.6	1.2	1.0	0.0	1.0	0.0	0.0

Table 188: Number of interactions between backbone atoms and hydrophobic side-chain atoms and average number of atom contacts at each position for interactions between pairs of α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	1	0	5	1	1	1	2	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.4	2.0	2.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	1	1	0	3	12	1	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	1.0	1.4	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	1	0	10	2	1	1	1	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.2	1.0	2.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 189: Number of interactions between backbone atoms and hydrophobic side-chain atoms and average number of atom contacts at each position for interactions between α -helices and β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	2	1	1	1	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	2.0	1.0	2.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 190: Number of interactions between backbone atoms and hydrophobic side-chain atoms and average number of atom contacts at each position for interactions between β -sheets and α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 191: Number of interactions between backbone atoms and hydrophobic side-chain atoms and average number of atom contacts at each position for interactions between pairs of β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	1	0	4	2	3	2	4	1	2	0	1	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	1.0	4.7	1.5	2.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	1	0	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	2.0	5.0	1.0	1.0	4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	1	2	0	1	4	2	2	0	0	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.5	0.0	1.0	1.8	2.5	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	1	0	1	2	8	3	13	8	25	9	10	7	2	0	1	1	0	1	0	0	0
90	120	0.0	0.0	0.0	0.0	1.0	0.0	1.0	1.5	1.2	1.7	1.8	2.2	1.9	1.9	1.3	2.0	1.0	0.0	3.0	2.0	0.0	1.0	0.0	0.0	0.0
120	150	0	0	1	1	1	3	7	6	24	11	40	13	59	24	26	7	11	6	3	1	6	1	0	0	0
120	150	0.0	0.0	2.0	2.0	2.0	1.0	1.7	1.2	1.6	1.8	1.3	1.6	1.6	1.5	1.4	1.0	1.7	1.8	2.0	1.0	1.7	1.0	0.0	0.0	0.0
150	180	0	1	0	0	1	3	15	10	26	8	39	9	67	29	34	11	16	8	5	3	1	0	0	0	0
150	180	0.0	2.0	0.0	0.0	1.0	1.3	1.6	1.3	1.7	1.2	1.2	1.6	1.4	1.2	1.2	1.5	1.4	1.2	1.0	2.3	1.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	4	3	11	4	17	6	32	14	16	10	8	1	2	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.3	1.3	1.2	1.2	1.8	1.8	2.1	1.4	1.2	1.1	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	1	2	1	7	2	5	4	8	1	1	1	4	0	2	1	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.5	1.0	1.0	1.0	3.2	1.8	1.4	2.0	1.0	2.0	1.0	0.0	2.5	3.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	2	0	3	4	6	1	1	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.5	0.0	1.7	1.2	1.7	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	2	3	4	2	8	3	9	3	5	1	0	2	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	1.5	1.3	1.8	2.5	1.5	1.3	2.0	1.7	1.4	2.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	1	1	3	0	1	0	7	1	6	4	4	0	4	1	2	1	0	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	1.0	2.0	1.0	0.0	1.0	0.0	1.3	1.0	1.2	1.2	1.2	0.0	1.2	1.0	1.5	1.0	0.0	0.0	0.0	0.0	0.0
-180	-150	0	1	0	1	3	5	7	6	10	3	13	7	30	12	21	7	13	7	7	4	3	0	1	0	0
-180	-150	0.0	1.0	0.0	1.0	1.3	2.2	1.7	2.2	1.7	1.0	1.4	1.0	1.3	1.5	1.8	1.3	1.4	1.7	1.6	1.2	1.0	0.0	1.0	0.0	0.0

Table 192: Number of interactions between hydrophobic side-chain atoms and average number of atom contacts at each position for interactions between pairs of α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	5	3	0	4	18	0	0	35	10	0	8	40	4	1	21	6	1	0	5	0	0	3	4	0
0	30	0.0	3.2	2.0	0.0	1.0	1.9	0.0	0.0	2.6	2.7	0.0	2.9	2.2	2.2	2.0	1.7	1.5	2.0	0.0	1.2	0.0	0.0	4.3	3.5	0.0
30	60	1	0	0	0	1	8	0	3	22	14	0	13	35	6	3	7	5	0	2	1	0	0	0	0	0
30	60	1.0	0.0	0.0	0.0	2.0	1.8	0.0	1.7	2.1	1.6	0.0	1.5	1.5	1.3	2.7	1.9	1.0	0.0	1.5	2.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	3	1	0	3	6	1	1	5	4	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.7	1.0	0.0	3.3	3.2	2.0	5.0	5.2	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	1	0	0	4	4	3	0	10	43	19	0	32	67	18	1	45	48	3	0	13	12	1	0	0	0
90	120	1.0	0.0	0.0	2.2	1.0	2.0	0.0	2.1	2.0	1.9	0.0	1.9	2.3	2.3	6.0	2.3	2.0	1.7	0.0	2.4	1.4	2.0	0.0	0.0	0.0
120	150	3	5	0	1	10	9	0	7	65	22	0	31	90	21	0	57	72	8	3	17	22	3	2	5	1
120	150	1.7	1.6	0.0	2.0	1.7	1.3	0.0	1.6	2.1	1.8	0.0	2.5	2.2	2.5	0.0	2.2	1.9	1.9	2.3	2.1	2.3	2.0	2.5	1.2	2.0
150	180	0	4	0	1	12	7	0	2	22	16	0	16	52	6	0	32	29	3	1	20	12	0	3	6	0
150	180	0.0	1.2	0.0	1.0	1.9	2.7	0.0	3.5	2.0	1.8	0.0	2.2	1.8	1.3	0.0	1.9	2.4	2.3	1.0	2.7	1.2	0.0	1.7	1.8	0.0
-30	0	0	1	0	0	3	4	0	0	19	2	0	11	33	5	0	18	15	3	0	10	9	2	0	3	2
-30	0	0.0	1.0	0.0	0.0	1.3	2.2	0.0	0.0	2.5	1.5	0.0	1.5	1.9	2.2	0.0	2.0	1.7	1.7	0.0	2.0	1.3	3.0	0.0	1.3	2.0
-60	-30	0	0	0	0	14	11	0	17	78	18	1	53	81	17	3	49	50	6	1	24	14	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	1.4	2.3	0.0	1.9	2.3	2.3	2.0	2.1	1.7	1.9	1.7	2.1	1.9	1.3	2.0	2.3	2.4	0.0	0.0	0.0	0.0
-90	-60	0	0	0	1	5	0	0	5	24	7	0	17	38	9	0	17	27	1	0	7	4	0	0	0	0
-90	-60	0.0	0.0	0.0	2.0	1.2	0.0	0.0	1.4	2.1	1.1	0.0	2.3	1.6	1.9	0.0	1.4	1.9	1.0	0.0	1.7	1.5	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	1	0	0	5	16	0	6	28	11	0	24	23	3	1	3	1	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	2.2	1.6	0.0	1.2	1.8	2.5	0.0	1.9	3.3	2.0	2.0	1.3	1.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	4	1	0	3	12	3	1	9	1	0	12	6	0	2	10	1	0	0	1	0
-150	-120	0.0	0.0	0.0	0.0	0.0	3.2	1.0	0.0	2.3	3.2	2.0	1.0	2.1	1.0	0.0	2.9	2.0	0.0	3.0	2.8	1.0	0.0	0.0	3.0	0.0
-180	-150	1	8	7	0	7	19	3	1	31	20	0	15	49	6	0	38	34	1	4	30	2	0	10	17	0
-180	-150	1.0	2.5	1.9	0.0	3.3	2.7	1.7	1.0	2.1	1.6	0.0	1.7	2.7	2.0	0.0	2.4	1.7	2.0	2.2	2.5	1.0	0.0	3.1	2.2	0.0

Table 193: Number of interactions between hydrophobic side-chain atoms and average number of atom contacts at each position for interactions between and α -helices β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	2	0	0	3	1	0	0	2	0	0	2	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	2.5	0.0	0.0	1.0	2.0	0.0	0.0	1.5	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	4	0	0	3	7	1	0	2	4	1	3	2	0	0	1	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.8	0.0	0.0	1.3	2.7	1.0	0.0	2.5	2.0	6.0	1.3	1.5	0.0	0.0	1.0	0.0	0.0
90	120	0	0	0	0	0	0	0	2	0	0	0	2	7	0	0	8	5	0	0	4	1	0	0	1	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.5	1.4	0.0	0.0	2.5	1.2	0.0	0.0	3.5	4.0	0.0	0.0	1.0	0.0
120	150	0	0	0	1	3	1	0	0	6	2	0	4	17	2	0	17	12	2	0	9	0	0	0	3	0
120	150	0.0	0.0	0.0	3.0	3.0	2.0	0.0	0.0	2.5	1.0	0.0	1.0	1.9	1.5	0.0	1.9	1.8	1.5	0.0	3.1	0.0	0.0	0.0	1.0	0.0
150	180	0	1	0	0	4	2	0	1	11	2	0	6	22	4	1	15	18	1	1	18	8	1	2	8	0
150	180	0.0	1.0	0.0	0.0	2.2	2.5	0.0	2.0	2.4	3.0	0.0	1.3	1.5	2.0	4.0	2.4	1.7	1.0	3.0	2.4	1.8	1.0	1.5	2.1	0.0
-30	0	0	0	0	0	0	1	0	0	1	1	0	2	8	1	0	3	5	0	0	2	1	0	0	1	0
-30	0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	3.0	1.0	0.0	4.5	2.3	7.0	0.0	3.7	1.4	0.0	0.0	3.0	2.0	0.0	0.0	1.0	0.0
-60	-30	0	0	0	0	2	1	0	0	4	1	0	0	3	1	0	2	3	0	0	1	3	0	0	1	0
-60	-30	0.0	0.0	0.0	0.0	2.0	1.0	0.0	0.0	1.8	2.0	0.0	0.0	1.0	2.0	0.0	1.5	3.0	0.0	0.0	2.0	1.3	0.0	0.0	2.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	1	0	0	1	2	0	0	0	1	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	****	2.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	1	2	0	2	3	0	0	3	1	0	1	2	0	0	4	1	0	1	2	0
-150	-120	0.0	0.0	0.0	0.0	0.0	2.0	2.5	0.0	1.5	1.7	0.0	0.0	1.7	2.0	0.0	1.0	7.0	0.0	0.0	5.5	1.0	0.0	2.0	2.0	0.0
-180	-150	0	0	0	0	0	0	0	0	0	0	1	1	6	1	1	3	4	0	1	3	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	5.2	1.0	1.0	2.3	2.8	0.0	3.0	1.3	0.0	0.0	0.0	0.0	0.0

Table 194: Number of interactions between hydrophobic side-chain atoms and average number of atom contacts at each position for interactions between β -sheets and α -helices.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	0	1	0	5	2	0	1	0	1	0	0	0	0	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	1.6	1.0	0.0	3.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	0	0	1	5	4	9	5	0	0	2	0	2	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.8	1.5	1.6	3.6	0.0	0.0	1.5	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	0	0	0	0	0	0	8	2	7	9	0	0	1	0	3	0	1	0	0	0	0	0
90	120	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.8	5.0	1.0	2.4	0.0	0.0	2.0	0.0	1.7	0.0	1.0	0.0	0.0	0.0	0.0	0.0
120	150	0	0	0	0	0	0	0	0	3	2	24	5	29	1	10	0	0	3	0	2	0	0	0	0	0
120	150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	2.5	1.2	1.8	2.0	1.8	0.0	0.0	3.3	0.0	3.0	0.0	0.0	0.0	0.0	0.0
150	180	0	0	0	0	0	0	2	2	11	7	37	4	40	6	12	5	0	0	0	0	0	0	0	0	0
150	180	0.0	0.0	0.0	0.0	0.0	0.0	1.5	3.5	2.1	1.0	2.2	2.2	1.7	2.8	2.2	1.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	0	0	0	0	0	6	0	8	0	6	0	4	0	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	0.0	2.5	0.0	2.7	0.0	2.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	1	0	2	0	4	0	9	0	4	0	2	0	0	0	0	0	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	1.5	0.0	1.8	0.0	1.9	0.0	1.8	0.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	0	0	0	0	0	1	2	0	2	0	0	0	0	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	7.0	0.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	0	1	3	0	0	4	0	4	5	0	3	0	0	0	1	0	1	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.3	0.0	0.0	4.8	0.0	4.8	1.4	0.0	2.3	0.0	0.0	0.0	1.0	0.0	4.0	0.0	0.0	0.0
-180	-150	0	0	0	0	0	0	0	0	1	0	6	0	6	1	6	0	1	0	0	0	0	0	0	0	0
-180	-150	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.8	0.0	4.8	4.0	2.3	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 195: Number of interactions between hydrophobic side-chain atoms and average number of atom contacts at each position for interactions between pairs of β -sheets.

ANGLE	RANGE	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
0	30	0	0	0	0	0	0	0	5	5	13	13	7	9	5	3	1	2	2	2	1	0	0	0	0	0
0	30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.8	1.8	2.3	2.2	1.9	1.9	1.6	1.7	5.0	3.5	1.5	1.0	1.0	0.0	0.0	0.0	0.0	0.0
30	60	0	0	0	0	0	0	2	1	3	1	3	2	0	2	0	0	0	0	0	0	0	0	0	0	0
30	60	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2.0	2.3	1.0	1.3	2.5	0.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
60	90	0	0	0	0	0	0	0	2	2	2	2	7	3	5	2	1	2	0	0	0	0	0	0	0	0
60	90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.5	1.5	2.5	2.5	2.0	4.0	2.2	1.0	5.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
90	120	0	0	0	1	1	0	5	6	10	16	18	26	22	18	18	10	5	2	0	1	1	2	0	0	0
90	120	0.0	0.0	0.0	1.0	3.0	0.0	1.8	2.3	2.8	2.2	2.5	1.9	1.3	2.3	1.8	5.0	1.6	2.0	0.0	1.0	1.0	2.0	0.0	0.0	0.0
120	150	0	0	1	2	1	7	11	12	26	54	53	81	83	74	66	35	32	16	8	9	6	2	0	1	0
120	150	0.0	0.0	2.0	4.0	1.0	1.0	2.6	1.9	2.2	2.0	1.6	2.2	2.2	2.2	2.1	1.9	1.9	2.4	1.6	1.8	1.0	1.0	0.0	2.0	0.0
150	180	2	2	1	1	5	8	12	21	30	60	60	86	91	76	82	39	39	20	17	6	4	0	0	0	0
150	180	1.0	1.0	1.0	1.0	2.2	2.5	1.5	1.6	2.1	2.2	2.3	2.0	2.3	2.1	2.2	1.9	2.3	2.0	1.4	1.7	3.5	0.0	0.0	0.0	0.0
-30	0	0	0	0	0	0	1	4	14	12	41	34	56	58	47	43	20	22	4	0	0	0	0	0	0	0
-30	0	0.0	0.0	0.0	0.0	0.0	2.0	1.2	2.3	1.3	2.3	2.6	2.2	2.1	2.4	2.0	1.8	1.5	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-60	-30	0	0	0	0	0	0	0	2	2	9	11	19	22	16	21	9	8	6	3	1	2	1	0	0	0
-60	-30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	2.0	2.2	1.7	2.0	3.1	2.1	2.1	2.4	1.2	1.0	4.0	3.0	0.0	0.0	0.0	0.0
-90	-60	0	0	0	0	0	0	0	0	0	5	4	9	10	6	4	0	0	0	0	0	0	0	0	0	0
-90	-60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.2	1.3	1.7	1.7	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-120	-90	0	0	0	0	0	0	2	2	4	14	6	12	12	10	9	4	3	1	1	0	0	0	0	0	0
-120	-90	0.0	0.0	0.0	0.0	0.0	0.0	2.5	1.0	1.0	1.6	2.5	1.7	2.0	2.5	1.8	1.2	2.7	1.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
-150	-120	0	0	0	0	0	4	1	6	5	7	5	7	9	5	6	8	8	5	0	1	1	0	0	0	0
-150	-120	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.8	1.4	2.1	4.6	3.3	3.9	2.2	4.8	1.9	1.5	1.2	0.0	1.0	1.0	0.0	0.0	0.0	0.0
-180	-150	0	0	3	3	1	7	9	19	18	28	22	34	26	25	24	21	21	17	14	10	8	2	3	1	0
-180	-150	0.0	0.0	2.3	1.7	1.0	1.6	1.7	3.0	1.9	2.7	1.9	2.1	3.2	1.9	1.8	2.7	1.9	3.1	2.3	1.4	1.6	1.5	1.7	3.0	0.0

APPENDIX L

Table 196. Number of occurrences of interactions between Ala β -carbons (position -4) and residues with hydrophobic side-chains at positions relative to nearest backbone contacts. Interactions are between two α -helices with crossing angles between -150° and -180° . Average number of atom contacts are included.

[illegible]

Table 197. Number of occurrences of interactions between Ala β -carbons (position -3) and residues with hydrophobic side-chains at positions relative to nearest backbone contacts. Interactions are between two α -helices with crossing angles between -150° and -180° . Average number of atom contacts are included.

	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
POSITION 12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
POSITION 11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
POSITION 10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 10	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
POSITION 9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
POSITION 8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
POSITION 7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
POSITION 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
POSITION 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
POSITION 4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
POSITION 3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
POSITION 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
POSITION 1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
POSITION 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
POSITION 0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0

Table 198. Number of occurrences of interactions between Ala β -carbons (position 0) and residues with hydrophobic side-chains at positions relative to nearest backbone contacts. Interactions are between two α -helices with crossing angles between -150° and -180° . Average number of atom contacts are included.

[illegible]

Table 199. Number of occurrences of interactions between Ala β -carbons (position +3) and residues with hydrophobic side-chains at positions relative to nearest backbone contacts. Interactions are between two α -helices with crossing angles between -150° and -180° . Average number of atom contacts are included.

[illegible]

Table 200. Number of occurrences of interactions between Ala β -carbons (position +4) and residues with hydrophobic side-chains at positions relative to nearest backbone contacts. Interactions are between two α -helices with crossing angles between -150° and -180° . Average number of atom contacts are included.

[illegible]

Table 201. Number of occurrences of interactions between Ala β -carbons (position +7) and residues with hydrophobic side-chains at positions relative to nearest backbone contacts. Interactions are between two α -helices with crossing angles between -150° and -180° . Average number of atom contacts are included.

[illegible]

Table 202. Number of occurrences of interactions between Ala β -carbons (position +11) and residues with hydrophobic side-chains at positions relative to nearest backbone contacts. Interactions are between two α -helices with crossing angles between -150° and -180° . Average number of atom contacts are included.

[illegible]

APPENDIX M

Table 203. Ratios of atom contacts/atom for each residue type for interactions between hydrophobic side-chain atoms. Ratios are for total protein interactions.

BROOKHAVEN FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
1HMD	113	898	6.16	0.87	1.75	0.17	0.50	1.00	0.80	1.50	0.00	4.14	3.89	2.80	1.87	7.00	4.29	1.00	0.75	1.88	4.87	5.00	5.00
1PCY	89	588	5.72	1.00	0.00	1.50	1.00	5.00	2.00	0.88	0.00	5.50	6.00	4.17	1.83	5.00	5.29	2.20	0.83	1.50	6.00	0.00	3.89
2CAB	258	1450	5.66	1.50	3.00	1.06	1.00	4.00	1.00	1.38	0.00	3.38	5.00	4.60	1.22	4.00	5.91	1.94	1.03	2.07	4.62	6.87	3.71
1CA2	258	1448	5.65	2.08	3.29	1.80	0.95	4.00	1.08	1.38	0.00	2.73	5.00	4.23	1.43	4.00	5.25	2.08	1.24	2.17	4.50	6.29	4.08
3DFR	162	900	5.58	1.53	1.50	1.80	0.54	0.00	1.00	1.29	0.00	2.14	4.80	4.21	1.22	5.50	5.50	0.88	0.75	2.21	4.80	6.25	3.82
3BLM	257	1420	5.53	2.78	3.25	1.14	1.67	0.00	1.25	1.88	0.00	1.00	5.11	5.00	1.40	5.33	6.43	3.00	1.32	2.82	3.77	0.00	4.31
2CPP	405	2210	5.48	1.83	2.42	0.75	1.41	3.12	0.88	1.38	0.00	2.89	4.58	4.71	1.33	4.20	6.22	1.37	0.83	1.82	3.89	6.80	3.79
2FCR	173	934	5.40	1.71	3.00	2.00	0.91	3.50	2.00	1.00	0.00	3.00	4.62	5.67	0.91	5.00	6.20	2.10	2.00	2.00	4.00	5.87	3.85
2PTC	281	1508	5.37	2.00	2.00	1.11	1.25	3.50	1.91	1.33	0.00	3.67	5.00	4.58	1.87	3.67	4.57	2.17	1.08	1.82	3.57	6.25	4.11
4FXN	138	738	5.35	2.87	1.00	0.38	0.22	4.00	1.00	1.28	0.00	0.00	4.60	5.25	1.80	4.80	6.80	2.87	1.00	0.80	3.87	3.87	3.70
1PPD	212	1134	5.35	2.21	1.92	0.82	1.33	2.57	1.48	1.57	0.00	5.00	5.00	4.82	2.40	0.00	5.25	1.50	1.85	2.25	3.00	4.80	3.89
1LYD	164	872	5.32	1.73	1.82	0.87	0.80	3.50	0.80	1.75	0.00	2.00	5.10	4.25	0.92	4.20	4.60	0.33	1.33	1.09	3.87	5.87	3.00
2TSC	264	1394	5.28	1.79	1.85	0.82	0.95	3.00	1.44	1.23	0.00	2.91	4.12	4.32	1.45	5.00	4.31	2.29	1.00	2.38	3.89	5.43	3.85
1RBP	174	912	5.24	2.48	1.00	0.75	1.35	2.50	0.88	0.22	0.00	3.50	4.75	2.87	2.50	3.25	5.20	1.00	0.80	1.87	4.88	4.50	3.08
1GP1	183	952	5.20	1.11	1.50	1.27	1.67	1.75	2.00	1.46	0.00	2.00	5.17	4.57	1.71	5.00	4.77	1.79	0.78	1.00	4.25	4.00	3.50
1APB	305	1580	5.18	1.90	1.88	1.00	1.24	5.00	1.45	1.55	0.00	4.33	5.44	4.95	1.80	4.80	5.50	1.93	1.50	1.94	4.33	5.80	3.54
3CLA	213	1094	5.14	1.91	2.22	0.50	0.50	4.25	1.20	0.70	0.00	2.14	5.09	4.15	0.87	4.17	3.82	2.44	0.87	1.45	3.80	5.33	3.25
1GCT	240	1232	5.13	1.73	1.87	1.00	1.89	3.40	1.70	2.20	0.00	2.00	4.70	4.67	1.29	3.50	5.00	3.00	1.12	1.88	3.20	5.82	4.04
2PAZ	123	828	5.09	1.84	3.00	0.57	1.00	5.00	1.00	1.10	0.00	5.00	4.27	5.00	1.08	4.40	6.33	1.88	1.00	0.80	4.75	0.00	3.83
1TON	227	1148	5.06	2.42	2.20	0.83	1.23	3.80	3.00	0.73	0.00	3.29	4.07	4.85	1.25	4.40	3.50	1.93	1.73	2.08	2.57	4.75	3.50
2RSP	228	1148	5.03	2.33	1.35	1.33	1.08	6.50	0.50	1.58	0.00	1.75	4.22	4.59	0.83	3.08	2.00	2.38	1.84	1.71	2.50	6.75	4.38
1CHO	291	1480	5.02	1.50	2.25	0.89	1.45	3.12	1.80	2.00	0.00	2.00	4.80	4.38	1.58	4.00	4.75	2.58	1.10	1.77	3.88	6.50	4.11
2APR	325	1628	5.01	1.87	0.88	1.00	1.18	2.75	1.55	2.12	0.00	0.00	4.61	5.32	1.92	5.00	5.59	1.75	0.88	1.82	5.00	5.40	4.30
4PTI	58	290	5.00	1.17	1.67	1.87	0.50	2.83	2.00	0.50	0.00	0.00	2.50	2.50	0.50	2.00	4.75	1.75	0.00	1.87	3.75	0.00	1.00
1CSC	429	2132	4.97	1.20	2.00	0.85	1.47	4.00	1.35	1.72	0.00	3.50	4.29	4.13	0.76	3.84	5.08	2.27	1.10	1.45	4.11	5.22	3.29
1TLD	223	1102	4.94	1.79	3.00	1.08	1.17	3.42	1.80	2.25	0.00	4.00	5.00	4.38	2.07	4.50	4.33	2.38	1.00	1.50	3.80	5.25	3.94
2GBP	309	1524	4.93	1.95	2.50	1.23	1.28	0.00	2.27	1.58	0.00	2.87	5.00	5.00	1.55	5.33	6.29	1.70	0.87	2.33	4.57	5.80	4.35
3APP	323	1590	4.92	2.25	0.00	1.27	1.48	2.00	1.44	1.00	0.00	1.87	4.92	5.10	2.40	0.00	5.20	1.75	0.72	1.83	4.43	6.87	4.98
1CCR	111	542	4.88	1.11	2.00	1.17	1.75	2.50	1.50	1.17	0.00	3.50	4.00	4.12	1.23	3.00	4.25	1.33	1.00	1.50	4.50	8.00	2.67
1BBP	173	838	4.83	1.88	1.00	1.18	1.30	3.25	2.00	1.08	0.00	2.33	3.71	4.83	1.50	0.00	4.80	1.50	1.42	1.14	3.81	4.40	2.95
2TIM	249	1188	4.77	1.88	2.30	1.00	0.82	2.00	1.38	1.82	0.00	3.80	4.74	4.29	1.12	2.00	5.25	1.88	0.83	1.33	3.40	6.80	3.78
1MBA	146	892	4.74	1.07	1.75	1.00	0.50	0.00	2.00	1.80	0.00	4.00	4.75	4.45	1.55	4.33	4.87	1.50	1.08	0.50	0.00	6.50	3.90
2C2C	112	530	4.73	1.20	0.00	1.00	0.87	2.00	1.00	1.00	0.00	4.00	4.50	3.88	1.18	5.00	4.20	2.33	2.00	0.82	5.80	7.00	3.50

Table 203. Ratios of atom contacts/atom for each residue type for interactions between hydrophobic side-chain atoms. Ratios are for total protein interactions (continued).

BROOKHAVEN FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
TTMN	318	1498	4.70	2.00	2.40	1.16	1.04	0.00	1.38	2.82	0.00	3.50	4.39	4.08	2.09	4.50	5.10	2.00	1.35	1.32	3.48	4.75	3.36
21BI	151	708	4.66	2.40	1.67	1.11	1.25	3.00	0.75	1.09	0.00	1.00	3.20	4.67	2.00	4.33	4.69	1.29	1.21	1.67	3.75	4.00	3.91
1SGT	223	1042	4.67	1.83	1.11	0.40	1.67	4.00	1.55	1.71	0.00	3.00	5.56	5.25	2.57	5.00	5.17	2.00	0.79	1.33	3.76	5.50	3.66
1TGS	281	1296	4.62	2.00	2.00	1.00	1.50	3.17	1.62	1.75	0.00	4.33	4.69	4.38	1.58	5.00	5.33	2.38	1.02	1.25	4.17	5.75	3.95
4PEP	326	1500	4.60	1.62	3.50	0.92	1.13	2.63	1.85	2.00	0.00	1.00	4.32	4.38	2.00	3.75	5.64	1.93	0.66	1.62	3.69	4.60	3.27
1CDP	108	498	4.59	0.80	1.00	1.33	0.57	2.00	0.50	1.33	0.00	5.00	5.20	4.67	1.08	0.00	5.90	0.00	0.80	1.40	0.00	0.00	3.20
1RNH	148	688	4.51	1.21	1.50	1.00	1.43	3.33	0.62	1.36	0.00	1.40	4.66	4.17	0.55	0.00	5.00	1.00	1.25	1.70	3.60	4.63	3.71
1SNC	135	598	4.43	2.00	2.40	2.40	2.33	0.00	0.60	2.55	0.00	1.50	4.40	4.64	1.05	3.75	5.00	1.50	1.00	1.38	3.43	4.00	4.67
351C	82	362	4.41	1.46	2.00	0.67	0.40	2.50	1.00	1.60	0.00	3.00	2.00	4.50	1.88	1.50	4.00	1.33	1.33	1.50	7.00	4.00	3.14
2SEC	338	1490	4.41	2.17	3.00	0.75	1.36	0.00	0.78	2.00	0.00	3.38	6.40	3.95	2.45	6.00	4.50	2.40	1.15	1.46	3.42	6.00	4.43
2HHB	574	2527	4.40	1.12	2.75	1.00	0.77	2.50	2.50	1.75	0.00	1.65	0.00	4.25	1.16	4.00	4.67	1.36	0.66	1.22	4.58	4.67	3.65
111B	152	688	4.39	2.00	0.67	0.67	0.66	3.50	0.42	1.06	0.00	1.00	2.80	4.20	1.93	4.00	4.69	1.57	1.00	2.00	3.50	4.00	3.62
1R69	63	276	4.36	1.50	1.25	0.33	0.00	0.00	1.33	2.25	0.00	0.00	3.67	5.11	1.40	0.00	7.00	1.50	0.29	1.25	0.00	3.00	4.75
1SAR	96	418	4.35	1.17	1.60	1.50	1.14	2.00	1.20	1.60	0.00	1.50	5.80	4.00	0.00	0.00	5.00	0.50	0.14	1.00	4.82	0.00	2.50
1UBQ	76	328	4.32	0.50	1.25	0.00	0.40	0.00	2.00	1.00	0.00	2.00	5.71	5.00	2.00	5.00	4.50	1.67	1.00	1.14	5.00	0.00	4.00
2PRK	279	1200	4.30	2.30	1.42	0.66	1.31	3.60	1.29	2.40	0.00	4.00	4.36	4.43	2.50	4.60	4.33	1.69	1.05	2.05	3.06	3.00	4.05
1CMD	107	480	4.30	1.67	1.00	1.50	0.60	2.00	0.67	1.11	0.00	1.00	4.67	5.75	1.57	3.67	5.62	2.50	0.40	1.60	1.50	0.00	5.00
3GRS	461	1982	4.26	1.92	1.62	0.59	1.10	2.67	1.00	1.14	0.00	1.50	4.24	4.35	1.53	3.47	4.29	1.66	1.19	1.94	4.15	6.33	3.39
1S02	275	1156	4.20	2.16	4.00	0.78	1.60	0.00	1.12	2.14	0.00	3.83	4.92	3.60	1.73	5.40	2.33	2.36	1.11	2.15	3.40	5.33	4.30
2OVO	56	234	4.16	0.50	2.00	0.40	1.50	2.33	0.00	1.00	0.00	1.00	0.00	3.50	2.50	0.00	4.50	1.33	0.60	0.75	3.00	0.00	2.75
1RSM	124	496	4.00	1.17	1.50	0.50	1.20	3.50	2.14	2.20	0.00	2.25	6.33	4.50	1.70	4.50	5.67	1.75	0.60	1.70	3.67	0.00	3.44
2CI2	65	256	3.97	2.67	2.25	0.50	1.25	0.00	0.00	1.43	0.00	0.00	3.00	3.33	1.67	0.00	5.00	2.00	2.00	1.67	1.00	6.00	2.60
1PAL	107	420	3.93	0.80	1.00	1.00	0.57	3.00	1.00	1.67	0.00	4.00	4.75	4.22	0.92	2.00	5.20	0.00	0.62	2.00	1.00	0.00	3.60
1HCE	74	280	3.78	2.14	1.67	2.00	0.60	3.00	2.00	1.25	0.00	1.50	1.50	2.75	4.00	0.00	0.00	1.67	0.60	1.12	2.33	2.00	4.68
1AAP	56	200	3.57	1.00	0.75	1.00	1.00	3.00	0.00	1.00	0.00	0.00	1.00	0.00	2.00	2.00	4.00	1.00	0.50	0.00	3.00	5.00	2.00
1CTF	66	232	3.41	1.80	3.00	1.00	0.75	0.00	0.00	1.11	0.00	0.00	4.00	4.29	1.50	0.00	3.00	0.00	0.00	3.00	0.00	0.00	4.36
3BCL	300	968	3.23	0.63	1.38	0.00	0.00	2.50	0.00	0.00	0.00	2.44	2.96	3.17	1.53	2.00	3.07	1.00	0.62	1.42	3.00	3.50	2.67
2RHE	114	346	3.05	1.44	1.00	1.33	1.14	5.00	1.80	0.80	0.00	0.00	4.20	3.30	1.00	0.00	3.00	0.75	0.29	1.25	4.00	4.00	2.67
256B	106	316	2.96	1.76	1.25	1.50	0.66	0.00	1.17	0.75	0.00	1.50	4.00	4.10	1.00	4.33	5.00	1.25	0.50	1.00	2.50	0.00	3.00
2UTG	70	206	2.97	0.50	1.50	0.50	0.50	1.50	0.50	1.00	0.00	1.00	2.75	2.25	1.57	2.00	2.50	1.00	0.60	1.00	5.00	0.00	1.33
2WRP	105	286	2.72	0.67	0.76	0.20	0.00	0.00	0.60	1.00	0.00	1.00	3.67	3.05	0.50	1.67	2.00	0.75	0.50	1.00	1.50	2.67	1.80
2MLT	26	34	1.31	0.00	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.33	1.75	0.67	0.00	0.00	0.00	0.00	0.50	0.00	1.00	0.00
1COX	502	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1BP2	123	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 204. Ratios of atom contacts/atom for each residue type for interactions between hydrophobic side-chain atoms. Ratios are for interactions between secondary structures.

BROOKHAVEN FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
1PCY	223	392	1.78	0.80	0.00	1.00	0.50	3.50	0.00	0.78	0.00	2.00	2.95	1.82	0.75	3.82	2.40	0.50	0.87	0.75	1.57	0.00	2.33
2FCR	316	498	1.57	2.10	1.12	0.50	0.00	3.50	0.00	0.87	0.00	2.25	2.29	2.31	0.22	1.25	1.84	2.27	1.75	2.00	0.29	1.56	2.42
3APP	818	968	1.58	2.47	0.00	0.82	0.94	1.00	1.02	0.87	0.00	0.00	1.73	2.10	0.38	0.00	1.95	0.83	0.88	1.18	1.51	2.11	2.47
3DFR	330	500	1.52	1.38	0.42	1.50	0.30	0.00	0.47	0.75	0.00	1.25	2.87	2.18	0.98	3.50	1.88	0.00	0.87	1.38	1.88	1.50	2.24
2RSP	472	700	1.48	1.75	0.82	0.87	0.33	5.75	0.00	1.33	0.00	0.00	1.81	2.12	0.88	1.40	1.00	1.82	1.20	1.08	1.00	0.00	2.00
1GCT	351	508	1.45	1.83	0.00	0.93	0.38	2.90	0.52	0.00	0.00	0.00	1.83	2.19	0.82	0.75	1.88	1.83	0.92	1.23	1.84	1.85	1.74
1TON	300	408	1.35	2.20	0.44	0.25	1.50	2.58	0.50	0.44	0.00	1.82	1.35	1.73	1.04	1.92	0.71	1.87	1.33	1.30	1.00	1.94	1.74
4FXN	290	388	1.34	3.20	0.25	0.10	0.00	5.00	0.50	0.84	0.00	0.00	1.84	2.45	0.41	1.75	1.81	1.17	1.50	0.87	1.14	0.78	2.00
1SGT	274	388	1.34	1.73	0.30	0.50	0.00	2.33	0.87	1.00	0.00	0.00	1.54	1.21	0.85	4.25	1.54	1.33	0.17	1.25	1.43	1.78	1.53
2PAZ	228	300	1.33	2.71	0.50	0.00	0.75	3.50	0.00	0.89	0.00	0.25	1.41	1.58	0.48	2.00	2.10	1.00	2.25	0.50	1.00	0.00	1.88
21BI	297	398	1.33	2.25	0.12	1.17	1.75	3.00	0.00	0.93	0.00	0.00	1.15	1.70	1.29	1.89	1.18	1.87	1.40	1.10	0.88	2.00	1.83
2PRK	483	810	1.32	2.08	0.92	0.00	0.58	3.00	0.53	0.00	0.00	2.08	2.08	1.23	1.30	1.75	1.57	2.22	0.88	0.88	0.74	1.28	2.53
2APR	520	888	1.32	2.87	0.38	0.75	0.81	1.50	0.73	1.00	0.00	0.00	1.25	1.78	0.15	2.25	1.80	0.87	0.50	0.88	1.30	1.58	2.24
1CDP	210	274	1.30	0.92	0.00	1.00	0.00	0.00	0.00	0.39	0.00	2.25	1.95	1.54	0.58	0.00	2.09	0.00	0.00	0.87	0.00	0.00	2.33
1LYD	405	522	1.29	3.14	0.84	0.84	0.58	2.00	0.33	0.82	0.00	1.00	2.58	1.73	0.31	1.50	1.88	0.00	1.00	0.71	1.40	1.89	1.48
1APB	838	828	1.29	2.75	0.53	0.58	0.89	4.50	0.44	0.74	0.00	2.00	2.13	1.85	0.74	1.53	1.59	0.87	1.09	1.05	0.83	1.80	1.74
1IIB	313	400	1.28	2.00	0.00	0.88	1.50	3.25	0.22	0.82	0.00	0.00	1.15	1.59	1.33	2.00	1.27	2.00	1.17	1.50	0.71	1.58	1.30
4PEP	599	738	1.23	1.71	0.82	0.50	0.91	3.17	0.80	0.47	0.00	0.00	1.89	1.49	0.75	1.25	1.88	0.13	0.71	0.48	0.79	1.18	1.87
2CPP	948	1140	1.21	2.20	0.49	0.17	0.57	2.20	0.17	0.39	0.00	1.43	1.81	1.85	0.72	2.21	1.92	0.84	1.23	1.75	1.07	1.88	1.87
1COX	895	844	1.21	2.00	1.14	0.17	0.70	0.00	0.58	0.84	0.00	4.00	1.34	1.59	0.29	1.72	1.51	0.00	0.50	1.47	1.27	1.14	1.91
1CHO	429	518	1.20	1.18	1.33	0.40	0.50	1.81	0.24	0.00	0.00	0.00	2.17	1.93	0.38	1.00	0.88	0.44	0.80	0.98	0.78	1.48	1.98
2CAB	408	484	1.19	1.85	0.89	1.00	0.50	1.50	0.47	0.33	0.00	1.04	1.48	1.71	0.19	1.75	2.21	0.53	0.82	0.75	0.71	0.94	1.98
1HOE	144	172	1.19	2.80	0.00	2.00	1.00	3.00	0.87	2.00	0.00	0.75	1.25	1.42	2.75	0.00	0.00	0.00	0.50	0.58	0.80	0.00	2.48
2GBP	803	712	1.18	2.03	0.80	0.50	0.31	0.00	1.24	0.44	0.00	0.58	2.23	1.38	0.48	1.35	1.57	0.83	0.40	1.50	0.95	1.87	1.85
1CA2	310	384	1.17	4.00	0.75	1.00	0.00	0.00	0.58	0.25	0.00	0.71	2.10	1.44	0.25	0.00	2.00	0.00	2.50	0.00	0.88	0.71	1.87
1TMN	525	808	1.18	2.71	1.35	0.38	0.25	0.00	0.24	1.22	0.00	1.25	1.80	1.47	0.58	2.50	1.33	1.00	1.08	0.75	0.84	1.44	1.58
1RNH	322	370	1.15	1.75	0.97	0.70	0.38	1.50	0.08	1.04	0.00	0.00	2.07	2.28	0.38	0.00	1.88	0.00	1.75	0.88	1.00	1.27	0.87
1HMD	238	272	1.15	1.00	0.50	0.00	0.00	2.00	0.50	0.42	0.00	1.88	1.60	1.15	0.17	2.00	2.78	0.00	1.00	1.38	0.50	2.58	0.50
1S02	352	400	1.14	2.00	1.50	0.42	0.25	0.00	0.33	0.75	0.00	1.30	1.81	1.29	0.48	1.58	0.00	1.33	0.58	1.10	0.57	0.87	1.81
2TIM	427	482	1.13	1.98	1.03	0.50	0.00	3.50	0.48	0.17	0.00	1.50	1.88	1.17	0.25	1.88	1.81	0.33	0.57	0.38	0.81	2.28	1.31
1CSC	1017	1152	1.13	1.77	0.43	0.30	0.88	1.87	0.87	0.54	0.00	0.98	1.85	1.43	0.35	1.48	1.33	1.03	1.18	0.73	1.18	1.54	1.47
2SEC	518	578	1.12	2.10	0.78	0.07	0.50	0.00	0.00	0.25	0.00	1.21	1.75	1.47	0.33	1.88	1.28	1.87	1.08	0.73	0.47	0.78	2.00
1PPD	303	340	1.12	2.87	1.44	0.33	0.12	0.75	0.20	1.89	0.00	0.75	1.17	1.42	0.50	0.00	1.48	1.83	1.20	0.75	0.78	0.78	1.79

Table 204. Ratios of atom contacts/atom for each residue type for interactions between hydrophobic side-chain atoms. Ratios are for interactions between secondary structures (continued).

BROOKHAVEN. FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
1UBQ	152	184	1.08	0.00	0.38	0.00	0.00	0.00	0.80	0.42	0.00	0.50	1.80	2.00	0.83	0.50	0.93	0.00	1.00	1.12	0.00	0.00	1.42
1RSM	254	274	1.08	0.80	0.33	0.28	0.83	3.42	0.61	0.78	0.00	0.31	2.08	1.25	0.46	1.62	1.14	1.22	1.33	1.25	1.14	0.00	1.44
1BP2	235	254	1.08	2.17	1.12	0.00	0.50	2.88	0.56	0.00	0.00	1.25	1.90	0.68	0.39	3.75	1.46	3.00	1.17	0.00	0.79	0.00	0.00
1MBA	338	380	1.07	0.80	0.81	0.83	0.21	0.00	0.67	0.53	0.00	0.25	1.44	1.33	0.53	1.33	1.57	0.22	1.11	0.75	0.00	1.56	1.25
1GP1	249	284	1.08	0.00	0.25	0.00	1.00	0.00	0.17	0.48	0.00	0.00	2.00	1.37	1.25	2.25	1.31	1.25	0.00	0.00	1.43	0.00	1.41
3GRS	979	1032	1.05	1.80	0.59	0.29	0.50	1.64	0.82	0.57	0.00	0.62	1.45	1.55	0.52	1.62	1.28	0.90	1.27	0.84	1.09	0.78	1.38
2RHE	180	184	1.02	1.88	0.12	0.00	0.00	4.25	1.11	0.00	0.00	0.00	1.55	1.20	0.25	0.00	0.50	0.00	0.11	0.50	1.38	2.33	0.67
1CMD	191	192	1.01	1.88	0.00	0.00	0.20	0.00	0.17	0.11	0.00	0.00	1.31	1.75	1.00	1.12	1.18	1.00	0.25	1.00	2.00	0.00	2.50
3CLA	452	452	1.00	2.88	0.38	0.00	0.20	1.75	0.46	0.29	0.00	0.20	1.83	1.32	0.71	1.15	0.78	2.56	1.12	0.67	1.31	0.56	1.48
1CTF	159	158	0.99	1.73	1.00	0.00	0.50	0.00	0.00	0.38	0.00	0.00	1.38	1.25	0.68	0.00	1.29	0.00	0.00	0.50	0.00	0.00	1.83
351C	124	120	0.97	1.38	0.00	0.00	0.00	0.50	0.33	0.58	0.00	0.00	1.50	1.50	0.20	0.00	1.68	3.33	0.00	2.50	1.43	1.58	1.33
4PTI	93	88	0.95	1.00	0.58	0.00	0.00	3.33	0.67	0.00	0.00	0.00	0.62	0.50	0.00	1.00	1.07	0.00	0.00	1.50	1.10	0.00	0.33
2CI2	117	110	0.94	1.00	0.67	0.00	0.17	0.00	0.00	0.22	0.00	0.00	1.75	1.17	0.67	0.00	0.71	1.17	0.00	1.50	0.00	1.44	1.29
1RBP	312	288	0.92	2.67	0.58	0.00	0.50	1.33	0.25	0.00	0.00	2.50	0.83	0.42	0.79	1.38	1.74	0.00	1.17	0.50	0.68	1.03	1.00
2HHB	1266	1108	0.88	1.05	0.97	0.28	0.61	1.58	0.54	0.57	0.00	0.89	0.00	1.23	0.11	1.81	0.91	0.79	0.85	0.73	1.20	0.93	1.37
1AAP	93	80	0.86	0.50	1.50	0.00	0.00	3.87	0.00	1.67	0.00	0.00	0.00	0.00	0.25	1.25	0.67	0.33	0.00	0.00	0.38	1.33	0.00
3BCL	698	594	0.85	0.87	0.53	0.00	0.00	2.00	0.00	0.00	0.00	1.08	1.24	1.38	0.82	0.44	0.72	0.47	0.64	0.79	1.00	0.67	1.00
1BBP	298	252	0.85	2.00	0.00	0.38	0.50	1.50	0.33	0.72	0.00	0.75	1.17	0.58	0.59	0.00	0.86	0.33	0.50	0.80	0.98	1.03	0.92
1SAR	119	100	0.84	1.00	0.62	0.00	0.17	0.50	0.00	0.42	0.00	0.25	2.17	0.94	0.00	0.00	0.00	0.00	0.00	0.88	0.80	0.00	2.33
1PAL	181	160	0.84	0.69	0.00	0.50	0.06	0.00	0.00	0.07	0.00	0.75	2.25	0.95	0.14	0.75	1.53	0.00	0.00	1.50	0.14	0.00	1.20
1R69	118	98	0.83	1.00	2.00	0.00	0.00	0.00	0.22	0.25	0.00	0.00	0.92	1.42	0.62	0.00	0.00	0.00	0.00	0.00	0.00	1.67	1.00
256B	242	162	0.67	2.21	0.42	0.80	0.06	0.00	0.20	0.11	0.00	0.00	1.33	1.22	0.22	1.08	0.57	0.00	0.00	0.75	0.21	0.00	1.17
1CCR	172	116	0.67	0.75	1.25	0.60	1.00	0.50	0.00	0.67	0.00	0.00	1.50	0.75	0.22	0.50	0.86	0.56	0.67	0.00	1.04	0.00	0.00
2UTG	138	74	0.54	0.00	0.00	0.25	0.00	0.00	0.00	0.42	0.00	0.50	0.50	1.38	0.35	0.75	0.00	0.00	1.00	0.10	2.00	0.00	0.17
2TSC	312	188	0.54	0.40	0.25	0.40	0.00	1.00	0.07	0.00	0.00	0.30	0.95	0.75	0.00	0.62	1.21	0.67	1.00	0.67	0.54	1.58	0.25
2PTC	176	92	0.52	0.80	0.83	0.17	0.00	1.90	0.33	0.00	0.00	0.00	0.25	0.00	0.17	0.75	1.00	0.00	0.00	0.83	0.60	0.00	0.67
2OVO	80	42	0.52	2.00	0.25	0.17	0.00	0.83	0.00	0.00	0.00	1.00	0.00	1.38	0.12	0.00	0.57	0.33	0.67	0.50	0.57	0.00	0.00
2C2C	183	80	0.49	0.40	0.00	0.00	0.00	0.00	0.00	0.82	0.00	0.00	1.50	0.12	0.12	1.50	0.29	0.00	2.33	0.00	0.57	0.00	1.50
1TGS	147	68	0.45	0.00	0.00	0.00	0.00	0.70	0.33	0.50	0.00	0.00	0.55	1.62	0.30	0.00	0.00	0.00	0.00	0.33	0.62	0.00	0.67
2WRP	261	104	0.40	0.40	0.08	0.00	0.00	0.00	0.27	0.18	0.00	1.12	0.92	0.77	0.42	0.00	0.00	0.00	0.50	0.17	1.29	0.00	0.27
1TLD	83	8	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.17	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.14	0.00	0.33
3BLM	415	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2MLT	77	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SNC	243	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 205. Ratios of atom contacts/atom for each residue type for interactions between oppositely charged atoms. Ratios are for total protein interactions.

BROOKHAVEN FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
1HOE	25	28	1.12	0.00	2.00	0.00	0.80	0.00	0.00	0.75	0.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CI2	36	38	1.06	0.00	1.62	0.00	0.75	0.00	0.00	0.84	1.33	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RBP	86	78	0.91	0.00	1.17	0.00	0.88	0.00	0.00	0.50	0.00	0.00	0.00	0.00	1.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RNH	67	60	0.90	0.00	1.30	0.00	0.93	0.00	0.00	0.77	0.00	0.00	0.00	0.00	0.36	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PPD	80	54	0.90	0.00	0.79	0.08	0.75	0.00	0.00	1.21	0.00	0.00	0.00	0.00	0.80	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SNC	65	58	0.89	0.00	1.80	0.00	1.17	0.00	0.00	0.88	0.00	0.00	0.00	0.00	0.82	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CPP	172	152	0.88	0.00	1.23	0.00	0.70	0.00	0.00	0.70	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1GP1	79	66	0.84	0.00	0.96	0.00	1.00	0.00	0.00	0.58	0.00	0.00	0.00	0.00	0.86	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2GBP	129	104	0.81	0.00	1.42	0.00	0.56	0.00	0.00	0.71	0.00	0.00	0.00	0.00	1.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1COX	149	116	0.78	0.00	1.15	0.00	0.80	0.00	0.00	0.67	0.00	0.00	0.00	0.00	0.83	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2SEC	65	50	0.77	0.00	1.00	0.00	0.50	0.00	0.22	0.62	0.05	0.00	0.00	0.00	0.82	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PRK	68	50	0.74	0.00	0.96	0.00	0.73	0.00	0.00	0.60	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2RHE	33	24	0.73	0.00	2.50	0.00	0.29	0.00	0.00	0.80	0.00	0.00	0.00	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1S02	49	36	0.73	0.00	1.50	0.00	0.25	0.00	0.12	0.86	0.00	0.00	0.00	0.00	1.09	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1APB	126	94	0.73	0.00	1.19	0.00	0.50	0.00	0.00	0.65	0.00	0.00	0.00	0.00	0.93	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2HHB	176	124	0.70	0.00	1.21	0.00	0.42	0.00	0.00	0.69	0.00	0.05	0.00	0.00	0.80	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SGT	57	40	0.70	0.00	0.44	0.00	0.56	0.00	0.00	0.84	0.00	0.00	0.00	0.00	0.08	1.71	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1R69	23	16	0.70	0.00	0.75	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CSC	126	82	0.65	0.00	0.74	0.00	0.50	0.00	0.00	0.67	0.00	0.00	0.00	0.00	0.72	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CDP	55	34	0.62	0.05	2.00	0.00	0.36	0.00	0.00	0.50	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TGS	59	36	0.61	0.00	1.12	0.05	0.69	0.06	0.00	0.31	0.00	0.00	0.00	0.00	0.47	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1LYD	75	46	0.61	0.00	0.69	0.00	0.35	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.39	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1HMD	49	30	0.61	0.00	0.62	0.00	0.42	0.00	0.00	0.62	0.00	0.00	0.00	0.00	1.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TMN	97	58	0.60	0.00	0.85	0.00	0.46	0.00	0.00	0.31	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3GRS	164	96	0.59	0.00	0.59	0.00	0.45	0.00	0.00	0.52	0.00	0.00	0.00	0.00	0.85	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2TIM	79	46	0.58	0.00	0.55	0.00	0.69	0.00	0.00	0.46	0.00	0.00	0.00	0.00	0.71	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2TSC	105	60	0.57	0.00	0.77	0.00	0.45	0.00	0.00	0.35	0.00	0.00	0.12	0.00	0.91	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3BLM	115	64	0.56	0.00	1.12	0.00	0.38	0.00	0.00	0.68	0.00	0.00	0.00	0.00	0.53	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
256B	61	34	0.56	0.00	0.38	0.00	0.29	0.00	0.00	0.62	0.00	0.00	0.00	0.00	1.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3CLA	82	44	0.54	0.00	0.83	0.00	0.38	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.58	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1IIB	61	32	0.52	0.00	0.50	0.00	0.19	0.00	0.00	0.54	0.00	0.00	0.00	0.00	0.87	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PAZ	44	22	0.50	0.00	0.00	0.00	0.10	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.92	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1UBQ	37	18	0.49	0.00	0.38	0.00	0.60	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.86	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 205. Ratios of atom contacts/atom for each residue type for interactions between oppositely charged atoms. Ratios are for total protein interactions (continued).

BROOKHAVEN FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
1MBA	45	22	0.49	0.00	0.75	0.00	0.19	0.00	0.00	0.80	0.00	0.00	0.00	0.00	0.45	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21BI	59	28	0.47	0.00	0.50	0.00	0.19	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.73	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RSM	38	18	0.47	0.00	1.00	0.00	0.50	0.00	0.00	0.40	0.00	0.00	0.00	0.00	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CTF	38	18	0.47	0.00	0.00	0.00	0.25	0.00	0.00	0.39	0.00	0.00	0.00	0.00	0.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CHO	64	30	0.47	0.00	1.12	0.06	0.36	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.29	0.00	0.00
4FXN	70	32	0.46	0.00	2.25	0.00	0.39	0.00	0.00	0.21	0.00	0.00	0.07	0.00	0.70	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2FCR	87	40	0.46	0.00	2.17	0.00	0.26	0.00	0.00	0.29	0.00	0.00	0.00	0.00	0.84	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.08
1CA2	101	46	0.46	0.00	0.79	0.00	0.45	0.00	0.00	0.23	0.00	0.00	0.00	0.00	0.52	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2RSP	102	44	0.43	0.00	0.40	0.00	0.50	0.00	0.00	0.12	0.00	0.00	0.00	0.09	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TON	74	32	0.43	0.00	0.70	0.00	0.19	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.56	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PAL	54	22	0.41	0.00	2.00	0.00	0.25	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.58	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1OMD	59	24	0.41	0.00	1.50	0.00	0.17	0.00	0.00	0.39	0.00	0.00	0.00	0.00	0.86	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3DFR	65	28	0.40	0.00	0.44	0.00	0.04	0.00	0.00	0.86	0.00	0.00	0.00	0.00	0.87	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
351C	30	12	0.40	0.00	0.50	0.00	0.30	0.00	0.00	0.30	0.00	0.00	0.00	0.00	0.82	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CAB	84	34	0.40	0.00	0.71	0.00	0.35	0.00	0.00	0.31	0.00	0.00	0.00	0.00	0.39	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2UTG	31	12	0.39	0.00	0.00	0.00	0.38	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.88	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2APR	87	34	0.39	0.00	0.29	0.00	0.25	0.00	0.00	0.38	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PCY	36	14	0.39	0.00	0.00	0.17	0.14	0.00	0.00	0.25	0.00	0.00	0.00	0.00	1.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1BBP	66	24	0.38	0.00	0.00	0.00	0.20	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.80	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PTC	62	22	0.35	0.00	0.31	0.11	0.44	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2WRP	54	18	0.33	0.00	0.44	0.00	0.12	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.87	0.00
1BP2	43	14	0.33	0.00	0.25	0.00	0.11	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.55	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CCR	37	10	0.27	0.00	0.00	0.00	0.00	0.00	0.00	0.42	0.00	0.00	0.00	0.00	0.38	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2C2C	47	12	0.26	0.00	0.00	0.00	0.17	0.00	0.00	0.22	0.00	0.00	0.00	0.00	0.35	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4PTI	24	6	0.25	0.00	0.25	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SAR	34	8	0.24	0.00	0.40	0.00	0.07	0.00	0.00	0.30	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3APP	59	10	0.17	0.00	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1GCT	48	8	0.17	0.00	0.87	0.00	0.17	0.00	0.00	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TLD	38	6	0.16	0.00	0.25	0.06	0.08	0.00	0.00	0.12	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4PEP	91	10	0.11	0.00	1.25	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3BCL	33	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2OVO	16	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2MLT	7	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1AAP	25	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 206. Ratios of atom contacts/atom for each residue type for interactions between oppositely charged atoms. Ratios are for interactions between secondary structures.

BROOKHAVEN FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
1HOE	13	12	0.92	0.00	0.67	0.00	1.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RNH	46	42	0.91	0.00	1.19	0.00	0.75	0.00	0.00	0.63	0.00	0.00	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1R69	16	12	0.75	0.00	1.00	0.00	0.00	0.00	0.00	0.75	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RBP	43	32	0.74	0.00	1.06	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.43	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1GP1	34	24	0.71	0.00	0.75	0.00	0.67	0.00	0.00	0.57	0.00	0.00	0.00	0.00	1.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1S02	24	14	0.58	0.00	1.50	0.00	0.38	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.67	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CI2	21	12	0.57	0.00	1.00	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1COX	67	32	0.48	0.00	0.61	0.00	0.30	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.38	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PCY	26	12	0.46	0.00	0.00	0.00	0.25	0.00	0.00	0.29	0.00	0.00	0.00	0.00	1.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3DFR	36	16	0.44	0.00	0.42	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TMN	52	22	0.42	0.00	0.70	0.00	0.38	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.67	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CPP	128	50	0.39	0.00	0.52	0.00	0.29	0.00	0.00	0.35	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CSC	95	36	0.38	0.00	0.46	0.00	0.32	0.00	0.00	0.35	0.00	0.00	0.00	0.00	0.38	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1MBA	41	14	0.34	0.00	0.50	0.00	0.00	0.00	0.00	0.70	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PAZ	24	8	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.67	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2FCR	42	14	0.33	0.00	1.50	0.00	0.25	0.00	0.00	0.21	0.00	0.00	0.00	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
256B	43	14	0.33	0.00	0.50	0.00	0.31	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.44	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3GRS	104	32	0.31	0.00	0.32	0.00	0.15	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.45	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CAB	33	10	0.30	0.00	0.82	0.00	0.50	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1BP2	33	10	0.30	0.00	0.25	0.00	0.00	0.00	0.00	0.63	0.00	0.00	0.00	0.00	0.57	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4FXN	42	12	0.29	0.00	1.25	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CA2	22	6	0.27	0.00	0.50	0.00	0.17	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2TSC	31	6	0.26	0.00	0.50	0.00	0.17	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1LYD	61	16	0.26	0.00	0.38	0.00	0.25	0.00	0.00	0.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21BI	24	6	0.25	0.00	0.00	0.00	0.25	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1BBP	24	6	0.25	0.00	0.90	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.38	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1APB	67	22	0.25	0.00	0.31	0.00	0.23	0.00	0.00	0.19	0.00	0.00	0.00	0.00	0.32	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2GBP	65	20	0.24	0.00	0.00	0.00	0.22	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.46	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PAL	33	6	0.24	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.57	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3CLA	44	10	0.23	0.00	0.21	0.00	0.00	0.00	0.00	0.36	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CDP	35	8	0.23	0.00	0.00	0.00	0.14	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.44	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CCR	27	6	0.22	0.00	0.00	0.00	0.00	0.00	0.00	0.30	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PRK	29	6	0.21	0.00	0.25	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 206. Ratios of atom contacts/atom for each residue type for interactions between oppositely charged atoms. Ratios are for interactions between secondary structures (continued).

BROOKHAVEN FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
1UBQ	20	4	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1H1B	30	8	0.20	0.00	0.00	0.00	0.17	0.00	0.00	0.14	0.00	0.00	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2UTG	21	4	0.19	0.00	0.00	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4PEP	47	8	0.17	0.00	1.00	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2HHB	120	20	0.17	0.00	0.00	0.00	0.17	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.31	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2C2C	28	4	0.14	0.00	0.00	0.00	0.17	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1HMD	28	4	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2TIM	49	8	0.12	0.00	0.12	0.00	0.30	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2SEC	38	4	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2RSP	54	8	0.11	0.00	0.11	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SAR	18	2	0.11	0.00	0.25	0.00	0.00	0.00	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
351C	21	2	0.10	0.00	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CHO	22	2	0.09	0.00	0.00	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PPD	28	2	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4PTI	10	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3BLM	51	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3BCL	33	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3APP	38	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2WRP	47	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2RHE	11	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PTC	15	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2OVO	8	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2MLT	7	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2APR	43	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TON	22	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TLD	5	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TGS	13	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SNC	39	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SGT	21	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RSM	24	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1OMD	29	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1GCT	18	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CTF	38	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1AAP	9	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 207. Ratios of atom contacts/atom for each residue type for interactions between atoms of like charge. Ratios are for total protein interactions.

BROOKHAVEN FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
1CDP	55	82	1.49	0.00	0.00	0.00	1.88	0.00	0.00	2.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PAL	54	70	1.30	0.00	0.00	0.00	1.54	0.00	0.00	2.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1OMD	59	58	0.98	0.00	0.25	0.00	1.27	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TMN	97	70	0.72	0.00	0.00	0.00	0.82	0.00	0.00	1.69	0.00	0.00	0.00	0.00	0.09	0.00	0.00	0.00	0.00	0.00	0.00	0.25	0.00
3APP	59	32	0.54	0.00	0.00	0.00	0.54	0.00	0.00	0.88	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2APR	87	38	0.44	0.00	0.00	0.00	0.64	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
351C	30	12	0.40	0.00	0.00	0.00	0.30	0.00	0.00	0.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RNH	87	24	0.38	0.00	0.30	0.00	1.00	0.00	0.00	0.09	0.00	0.00	0.00	0.00	0.18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2C2C	47	18	0.34	0.00	0.00	0.00	0.42	0.00	0.00	0.81	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
258B	81	20	0.33	0.00	0.12	0.00	0.42	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2GBP	129	38	0.29	0.00	0.17	0.00	0.40	0.00	0.00	0.38	0.00	0.00	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2FCR	87	24	0.28	0.00	0.33	0.00	0.28	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PCY	36	10	0.28	0.00	-0.00	0.00	0.21	0.00	0.00	0.44	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4PEP	91	24	0.26	0.00	0.00	0.00	0.32	0.00	0.00	0.19	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4FXN	70	18	0.26	0.00	0.00	0.00	0.28	0.00	0.00	0.34	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TLD	38	10	0.26	0.00	0.00	0.00	0.17	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CHO	84	18	0.25	0.00	0.00	0.00	0.41	0.00	0.00	0.19	0.00	0.00	0.00	0.00	0.22	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1APB	128	32	0.25	0.00	0.12	0.00	0.33	0.00	0.00	0.30	0.00	0.00	0.00	0.00	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1HMD	49	12	0.24	0.00	0.12	0.00	0.25	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PPD	80	14	0.23	0.00	0.29	0.08	0.08	0.00	0.00	0.14	0.00	0.00	0.00	0.00	0.30	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CI2	36	8	0.22	0.00	0.75	0.00	0.12	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2TSC	105	22	0.21	0.00	0.31	0.00	0.17	0.00	0.00	0.27	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RSM	38	8	0.21	0.00	0.25	0.00	0.10	0.00	0.00	0.10	0.00	0.00	0.00	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TGS	59	12	0.20	0.00	0.00	0.00	0.12	0.00	0.00	0.38	0.00	0.00	0.00	0.00	0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3BLM	115	22	0.19	0.00	0.38	0.00	0.22	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.28	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PTC	82	12	0.19	0.00	0.06	0.00	0.12	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1LYD	75	14	0.19	0.00	0.35	0.00	0.10	0.00	0.00	0.12	0.00	0.00	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3BCL	33	6	0.18	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2RSP	102	18	0.18	0.00	0.20	0.00	0.18	0.00	0.00	0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2RHE	33	6	0.18	0.00	0.00	0.00	0.07	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SAR	34	6	0.18	0.00	0.60	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1HOE	25	4	0.18	0.00	0.00	0.00	0.20	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CPP	172	28	0.15	0.00	0.21	0.00	0.23	0.00	0.00	0.06	0.00	0.00	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 207. Ratios of atom contacts/atom for each residue type for interactions between atoms of like charge.
Ratios are for total protein interactions (continued).

BROOKHAVEN FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
1BBP	68	10	0.15	0.00	0.00	0.00	0.20	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1GP1	79	10	0.13	0.00	0.04	0.00	0.17	0.00	0.00	0.19	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2SEC	65	8	0.12	0.00	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SNC	65	8	0.12	0.00	0.00	0.00	0.58	0.00	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1S02	49	6	0.12	0.00	0.00	0.00	0.15	0.00	0.00	0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1GCT	48	6	0.12	0.00	0.00	0.00	0.22	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SGT	57	6	0.11	0.00	0.00	0.00	0.17	0.00	0.00	0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CTF	38	4	0.11	0.00	0.00	0.00	0.25	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CSC	128	14	0.11	0.00	0.05	0.00	0.15	0.00	0.00	0.19	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3GRS	164	16	0.10	0.00	0.19	0.00	0.14	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3DFR	65	6	0.09	0.00	0.25	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PRK	68	6	0.09	0.00	0.00	0.00	0.19	0.00	0.00	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RBP	88	8	0.09	0.00	0.25	0.00	0.03	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1R69	23	2	0.09	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4PTI	24	2	0.08	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TON	74	6	0.08	0.00	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1COX	149	12	0.08	0.00	0.00	0.00	0.14	0.00	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1H1B	61	4	0.07	0.00	0.00	0.00	0.12	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2UTG	31	2	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1UBQ	37	2	0.05	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CCR	37	2	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2WRP	54	2	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CA2	101	4	0.04	0.00	0.00	0.00	0.05	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2TIM	79	2	0.03	0.00	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2HHB	176	6	0.03	0.00	0.00	0.00	0.05	0.00	0.00	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3CLA	82	2	0.02	0.00	0.00	0.00	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PAZ	44	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2OVO	16	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2MLT	7	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CAB	84	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21BI	59	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1MBA	45	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1BP2	43	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1AAP	25	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 208. Ratios of atom contacts/atom for each residue type for interactions between atoms of like charge.
Ratios are for interactions between secondary structures.

BROOKHAVEN FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
3APP	38	14	0.37	0.00	0.00	0.00	0.29	0.00	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2APR	43	14	0.33	0.00	0.00	0.00	0.44	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TMN	52	16	0.31	0.00	0.00	0.00	0.54	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1S02	24	6	0.25	0.00	0.00	0.00	0.38	0.00	0.00	0.38	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1GP1	34	8	0.24	0.00	0.08	0.00	0.50	0.00	0.00	0.21	0.00	0.00	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CDP	35	8	0.23	0.00	0.00	0.00	0.07	0.00	0.00	0.58	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SGT	21	4	0.19	0.00	0.00	0.00	1.00	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3BCL	33	6	0.18	0.00	0.22	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RNH	46	8	0.17	0.00	0.00	0.00	0.75	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2GBP	85	12	0.14	0.00	0.10	0.00	0.19	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
256B	43	6	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1APB	87	12	0.14	0.00	0.00	-0.00	0.31	0.00	0.00	0.15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4PEP	47	6	0.13	0.00	0.00	0.00	0.19	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1UBQ	20	2	0.10	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TON	22	2	0.09	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3GRS	104	8	0.08	0.00	0.27	0.00	0.04	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RSM	24	2	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PPD	26	2	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CSC	95	8	0.08	0.00	0.07	0.00	0.11	0.00	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
111B	30	2	0.07	0.00	0.00	0.00	0.17	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3DFR	36	2	0.06	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CTF	36	2	0.06	0.00	0.00	0.00	0.12	0.00	0.00	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2FCR	42	2	0.05	0.00	0.00	0.00	0.06	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CPP	128	6	0.05	0.00	0.00	0.00	0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2HHB	120	4	0.03	0.00	0.00	0.00	0.06	0.00	0.00	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1LYD	61	2	0.03	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4PTI	10	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4FXN	42	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3CLA	44	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3BLM	51	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
351C	21	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2WRP	47	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2UTG	21	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 208. Ratios of atom contacts/atom for each residue type for interactions between atoms of like charge.
Ratios are for interactions between secondary structures (continued).

BROOKHAVEN FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
2TSC	31	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2TIM	49	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2SEC	36	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2RSP	54	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2RHE	11	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PTC	15	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PRK	29	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PAZ	24	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2OVO	8	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2MLT	7	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CI2	21	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CAB	33	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2C2C	28	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21BI	24	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TLD	5	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TGS	13	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SNC	39	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SAR	18	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RBP	43	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1R69	16	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PCY	26	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PAL	33	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1OMD	29	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1MBA	41	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1HOE	13	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1HMD	28	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1GCT	18	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1COX	87	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CHO	22	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CCR	27	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CA2	22	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1BP2	33	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1BBP	24	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1AAP	9	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 209. Ratios of atom contacts/atom for each residue type for interactions between charged atoms and polar side-chain atoms. Ratios are for total protein interactions.

BROOKHAVEN FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
3APP	59	38	0.61	0.00	0.00	0.00	0.83	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CAB	84	46	0.55	0.00	0.57	0.00	0.77	0.00	0.00	0.58	0.00	0.00	0.00	0.00	0.11	0.00	0.09	0.00	0.00	0.00	0.00	0.00	0.00
2APR	87	45	0.52	0.00	0.36	0.00	0.86	0.00	0.00	0.44	0.00	0.00	0.00	0.00	0.31	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2SEC	65	33	0.51	0.00	0.50	0.00	0.45	0.00	0.11	0.62	0.03	0.00	0.00	0.00	0.27	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PPD	60	29	0.48	0.00	0.21	0.00	0.83	0.00	0.00	0.71	0.00	0.00	0.00	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TMN	97	46	0.47	0.00	0.20	0.00	0.52	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.36	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PRK	66	30	0.44	0.00	0.38	0.00	0.62	0.00	0.00	0.40	0.00	0.00	0.00	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SAR	34	15	0.44	0.00	0.30	0.00	0.50	0.33	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1BP2	43	17	0.40	0.00	1.00	0.00	0.56	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.09	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1HMD	49	19	0.39	0.00	0.00	0.00	0.42	0.00	0.00	0.88	0.00	0.00	0.11	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CA2	101	36	0.36	0.00	0.21	0.00	0.50	0.00	0.00	0.42	0.00	0.00	0.00	0.00	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1COX	149	52	0.35	0.00	0.28	0.00	0.42	0.00	0.00	0.43	0.00	0.00	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2TIM	79	26	0.33	0.00	0.40	0.00	0.25	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2RHE	33	11	0.33	0.00	0.25	0.00	0.36	0.00	0.00	0.30	0.00	0.00	0.00	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CPP	172	56	0.33	0.00	0.15	0.00	0.55	0.00	0.00	0.36	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1S02	49	16	0.33	0.00	0.00	0.00	0.50	0.00	0.12	0.21	0.00	0.00	0.00	0.00	0.18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3BLM	115	37	0.32	0.00	0.12	0.00	0.47	0.00	0.00	0.32	0.00	0.00	0.00	0.00	0.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1HOE	25	8	0.32	0.00	0.00	0.00	0.60	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PTC	62	19	0.31	0.05	0.31	0.00	0.31	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.39	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2GBP	129	40	0.31	0.00	0.42	0.00	0.35	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TGS	59	18	0.31	0.00	0.88	0.00	0.38	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.26	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CHO	64	20	0.31	0.00	0.25	0.00	0.50	0.00	0.00	0.38	0.00	0.00	0.00	0.00	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1R69	23	7	0.30	0.00	0.00	0.00	0.00	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4PEP	91	26	0.29	0.00	0.25	0.00	0.37	0.00	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21BI	59	17	0.29	0.00	0.50	0.00	0.19	0.00	-0.00	0.41	0.00	0.00	0.00	0.00	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TLD	38	11	0.29	0.00	1.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RSM	38	11	0.29	0.00	0.00	0.00	0.70	0.00	0.00	0.30	0.00	0.00	0.00	0.00	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CSC	126	36	0.29	0.00	0.21	0.00	0.38	0.00	0.00	0.36	0.00	0.00	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1LYD	75	21	0.28	0.00	0.19	0.00	0.45	0.00	0.00	0.31	0.00	0.00	0.00	0.00	0.15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2RSP	102	28	0.27	0.00	0.03	0.00	0.66	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2HHB	176	48	0.27	0.00	0.21	0.00	0.35	0.00	0.00	0.36	0.00	0.00	0.00	0.00	0.09	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1BBP	66	16	0.27	0.00	1.50	0.00	0.35	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1SNC	65	17	0.26	0.00	0.00	0.00	0.58	0.00	0.00	0.41	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 209. Ratios of atom contacts/atom for each residue type for interactions between charged atoms and polar side-chain atoms. Ratios are for total protein interactions (continued).

BROOKHAVEN FILE-NAME	TOTAL RESIDUES	TOTAL CONTACTS	TOTAL	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
1SGT	57	15	0.26	0.00	0.28	0.00	0.28	0.00	0.00	0.29	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2TSC	105	26	0.25	0.00	0.08	0.00	0.40	0.00	0.00	0.19	0.00	0.00	0.08	0.00	0.09	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2OVO	16	4	0.25	0.00	0.00	0.00	0.50	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3BCL	33	8	0.24	0.00	0.19	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1TON	74	18	0.24	0.00	0.50	0.00	0.19	0.00	0.00	0.32	0.00	0.00	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RNH	67	16	0.24	0.00	0.10	0.00	0.43	0.00	0.00	0.36	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
256B	61	14	0.23	0.00	0.12	0.00	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1GCT	48	11	0.23	0.00	0.33	0.00	0.33	0.00	0.00	0.30	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1APB	128	30	0.23	0.00	0.08	0.00	0.31	0.00	0.00	0.35	0.00	0.00	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PCY	36	8	0.22	0.00	0.00	0.00	0.43	0.00	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1GPI	79	17	0.22	0.00	0.07	0.00	0.44	0.00	0.00	0.27	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CCR	37	8	0.22	0.00	0.75	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3GRS	164	34	0.21	0.00	0.28	0.00	0.24	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1RBP	86	18	0.21	0.00	0.12	0.00	0.32	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1HB	61	13	0.21	0.00	0.00	0.00	0.25	0.00	0.00	0.38	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3DFR	65	12	0.18	0.00	0.19	0.00	0.19	0.00	0.00	0.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4PTI	24	4	0.17	0.00	0.17	0.00	0.25	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1PAL	54	9	0.17	0.00	0.50	0.00	0.18	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2UTG	31	5	0.16	0.00	0.50	0.00	0.12	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2FCR	87	14	0.16	0.00	0.00	0.00	0.28	0.00	0.00	0.04	0.00	0.00	0.00	0.00	0.09	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1MBA	45	7	0.16	0.03	0.12	0.00	0.08	0.00	0.00	0.30	0.00	0.00	0.00	0.00	0.09	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CDP	55	9	0.16	0.00	0.00	0.00	0.21	0.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1OMD	59	9	0.15	0.00	0.00	0.00	0.17	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2PAZ	44	6	0.14	0.00	0.00	0.00	0.10	0.00	0.00	0.15	0.00	0.00	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2MLT	7	1	0.14	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2CI2	36	5	0.14	0.00	0.00	0.00	0.25	0.00	0.00	0.07	0.33	0.00	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3CLA	82	11	0.13	0.00	0.08	0.00	0.25	0.00	0.00	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1AAP	25	3	0.12	0.00	0.12	0.00	0.25	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4FXN	70	8	0.11	0.00	0.25	0.00	0.11	0.00	0.00	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2WRP	54	6	0.11	0.00	0.08	0.00	0.12	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.87	0.00
1UBQ	37	4	0.11	0.00	0.00	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
351C	30	3	0.10	0.00	0.00	0.00	0.10	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2C2C	47	2	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1CTF	38	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

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