CH··O hydrogen bonds at protein-protein interfaces

Lin Jiang and Luhua Lai*

State key Laboratory for Structural Chemistry of Stable and Unstable Species,

Beijing 100871, China

Institute of Physical Chemistry, Department of Chemical Biology, College of Chemistry, Peking University, Beijing 100871, China

Center for Theoretical Biology, Peking University, Beijing 100871, China

* Corresponding author

Email:  lhlai@pku.edu.cn or lai@mdl.ipc.pku.edu.cn

Fax: 086-10-62751725

Phone: 086-10-62757486

Key words: hydrogen bonds; C-H··O hydrogen bonds; pair potentials; knowledge-based potentials; protein-protein interaction; protein recognition.
[ABSTRACT]

For the first time a statistical potential has been developed to quantitatively describe the CH···O hydrogen bonding interaction at the protein-protein interface. The calculated energies of CH···O pair interaction show a favorable valley at about 3.3Å, exhibiting the feature typical of hydrogen bond and is similar to the ab initio quantum calculation result (39). The potentials have been applied to a set of 469 protein-protein complexes to calculate the contribution of different types of interactions for each protein complex: the average energetic contribution of conventional hydrogen bond is around 30%; that of CH···O hydrogen bond is 17% and hydrophobic interaction is 50%. In some protein-protein complexes the contribution of the CH···O H-bond can reach as high as 40~50%, indicating the importance of the CH···O H-bond at the protein interface. At the interfaces of these complexes, CαH···O H-bonds frequently occur between adjacent strands in both parallel and anti-parallel orientation, having the obvious structural motif of the bifurcated hydrogen bonds. Our study suggests that the CH···O weak hydrogen bond provides important contribution to the association and stability of protein complexes and needs more attention in protein-protein interaction studies.
[INTRODUCTION]

The conventional hydrogen bonds of the type X—H···Y (X, Y= N or O) have been widely found and thoroughly studied in macromolecular structures, from both experimental and theoretical perspectives (1, 2, 7-9). On the other hand, close CH···O contacts occur often in protein structures and are considered as hydrogen bonds. It is increasingly recognized that weak CH···O hydrogen bonds play an important role in the stabilization and the function of biological macromolecules (3-6).

CH···O contacts are now having increasingly wide acceptance as a genuine hydrogen bond (10, 11). Much of the evidence for the CH···O hydrogen bond comes from the observation that short intermolecular CH···O contacts are well established in many small molecule crystals (12, 13). In more recent years neutron diffraction studies of amino acid crystals, which yield highly accurate positions of hydrogen atoms experimentally, provide convincing evidences in favor of the ability of the carbon atoms to function as hydrogen bond donors in CH···O contacts directly (14). Recently there are surveys of high-resolution protein structures that reveal the widespread occurrence of CH···O weak hydrogen bonds (15-21, 59, 60). Hereinto various studies have reported the existence of a CαH···O weak hydrogen bond between the parallel β-sheets in proteins (17, 59, 60). At the same time, some mutation studies on protein-ligand interactions have reported that the CH···O weak bonds are proved to stabilize the protein-ligand complexes (10, 22, 23). Similar to protein-ligand interfaces, close CH···O contacts abound at protein-protein interfaces. Although CH···O H-bonds are normally weaker than conventional hydrogen bonds, their number cannot be neglected. The CH···O hydrogen bonding interaction is also thought to be important for the interactions of nucleic acids with proteins and drug binding (24-26), and thus it would be surprising if CH···O interactions were less important in protein interfaces. In fact, the CH···O hydrogen bonding interaction has been considered so important that many crystal refinement programs that treat CH···O contacts as repulsive have been called into question (10, 27, 28).
However the energetic contribution of this kind of interactions to the stability of protein-protein complexes as compared to other forces remains to be explored. Despite the finding of numerous CH···O contacts at protein-protein interfaces, it remains unclear about their relative importance in the protein recognition or drug binding process. Although some structural analyses have provided a wealth of information about average hydrophobicities and residue compositions of protein-protein complexes (29-33), they did not provide any quantitative information on the strengths of these different sorts of interactions (such as hydrophobic interaction, hydrogen bonding interaction and CH···O hydrogen bonding interaction). But it is the quantitative magnitude of the interaction that is of most significance in understanding the possible role each of them plays in the association of protein complex.

In attempts to describe the energetic aspects of CH···O interactions, theoretical calculations have been developed to evaluate the strength of CH···O interactions (34-37). *Ab initio* quantum calculation has shown that a small molecule such as CH$_2$F$_2$ can establish an H-bond of the strength similar to a conventional OH···O interaction (38). Recently the *ab initio* quantum calculation for the C$^\alpha$H···O hydrogen bond of some representative amino acid residues (39) has demonstrated that the peptide CH group is a potent proton donor and the CH···O interaction appears to be a true hydrogen bond. Furthermore the study also shows that some CH···O bond is even stronger than a conventional OH···O interaction, suggesting that the CH···O hydrogen bond interactions in proteins need to be paid more attention.

*Ab initio* quantum calculation (39) gave a series of calculated binding strengths for the C$^\alpha$H···O contacts of different amino acid residues in an ideal model. However the energetic percentage of CH···O interaction is still not known (i.e. what ratio of CH···O interaction in the total binding energy of protein complexes is). Thus the relative importance of CH···O interaction in the protein association remains somewhat an open question.
Here for the first time we calculate the average energetic percentage of CH⋯O interaction in total binding free energy, using our established mean-field potential for describing protein-protein complexes (40). The potentials of mean force (PMF), a beneficial tool in protein fold recognition, generally use the training database of known protein structures to extract ‘pseudo-potentials’ for predicting unknown structures (46-49). Many applications have demonstrated their usefulness in studies of protein-ligand binding (50-55) and in protein-protein associations (56-57).

Based on the new definition of atom types and our developed method, the distance dependent potentials have been derived to describe different types of interactions at the protein-protein interface. And the energetic aspects of CH⋯O interactions have been discussed quantitatively. The calculated energies of CH⋯O pair interactions exhibit the feature typical of hydrogen bond. The quantitative study on the energetic percentage have shown the importance of the CH⋯O hydrogen bond at the protein interface. The obvious structural motif of bifurcated hydrogen bond is highlighted in the stereochemical analysis of CH⋯O contacts in the representative examples with a high CH⋯O percentage. We expect that the method would be helpful to understand the interactions in protein-protein interfaces and how they drive protein-protein associations.

[METHOD]

We use the established empirical approach for the description of protein-protein association from energetic aspect. The mean-field potentials are derived from the same training set as that used before (40). Using the methodology as described in our previous paper, we implicitly treat solvation and entropic effects and directly estimate total free binding energies of protein-protein complexes without any knowledge of experimental binding affinities and fitting procedures.

1. New definition of five atom types
To extract and characterize the CH···O hydrogen bonding interactions, five atom types are defined: hydrogen bond donor (D), hydrogen bond acceptor (A), both donor and acceptor (B), CH type—neutral atom bonded to hydrogen atoms (CH), and neutral type—neither donor nor acceptor (N). In the atom type definition, primary and secondary amines are defined to be donors; oxygen and nitrogen atoms with no bound hydrogen are defined to be acceptors; hydroxyl oxygen, ND NE of HIS and carboxyl oxygen in C-terminal are defined to be both donor and acceptor; carbon atoms with hydrogen atom are defined to be CH type; and carbon atoms with no bound hydrogen and sulfur atoms are defined to be neither donor nor acceptor. The atom occupancy in the crystal structure file is used to function as a weighting factor.

The distance-dependent Helmholtz free energies of protein-protein complexes are extracted from the non-redundant training set (40) in Brookhaven Protein Data Bank (43, 44). Atoms of the ‘receptor’ part and the ‘ligand’ part are treated differently. So we calculate 25 atom pair interaction terms here (see Table 1). In our training set metal and hetero-atoms are excluded. It is assumed that all crystallized complexes use water as the medium. Water molecules are neglected, as the solvation effects are implicitly treated. Hydrogen atoms are omitted in all the analysis.

2. Statistical potentials

Pair potentials are derived from the training set using the same methodology described in the previous paper (40). Here we only give a brief description of the method.

According to reverse Boltzmann relationship, the free energy between the ‘receptor’ atom of type i and the ‘ligand’ atom of type j at a distance r can be written as

\[ A_{ij} = -kT \ln[f_{ij}(r)/Z_{ij}] \]  

(1)

where \( k \) is the Boltzmann constant and \( T \) is the absolute temperature. \( f_{ij}(r) \) is a frequency of these ij contacts occurring at distance r. In fact, our statistical potential \( \Delta A_{ij}(r) \) is the difference relative to a reference potential.
\[ A_{ij} - \text{reference energy} = \Delta A_{ij}(r) = kT \ln[1 + m_{ij} \sigma] - kT \ln[1 + m_{ij} \frac{g_{ij}(r)}{f(r)}] \] (2)

where \( m_{ij} \) is the total number of contacts between types i and j, \( g_{ij}(r) \) is the distribution of these contacts occurring at distance \( r \), \( f(r) \) is the distribution of all contacts for all types at distance \( r \). The atom pair distance \( r \) uses a histogram-based representation, and \( r \) here refers to a given bin of width 0.2 Å. We simplify our reference energy: we just import a big value in very short distance (i.e. where our statistics are not included), in order to capture strong \textit{van der Waals} repulsive potentials in this distance range.

The derived potentials for the interaction of ‘receptor’ atom type i and ‘ligand’ atom j are summed up to evaluate the total PMF value.

\[
A = \sum \Delta A_{ij}(r) \times \Delta g
\] (3)

\[
\begin{align*}
\Delta g &= 0 & \text{for} & r > r_{\text{cut-off}} \\
\Delta g &= p_i \times p_j & \text{for} & r \leq r_{\text{cut-off}}
\end{align*}
\]

For atom presentations, occupancy ratio \( p_i \) is used to function as a weighting coefficient.

The occurrence of the atom pair in a distance less than 8.0 Å is recorded. If the total number of atom pairs in the shell of a distance \( r \pm \Delta r \) (\( \Delta r = 0.1 \) Å) is less than 30, the contributions of all atom pairs at the distance interval are ignored because of their statistically insufficient data.

3. The contribution of different interactions to the total binding free energy in each protein-protein complex

We apply the statistical potentials to a larger set of protein-protein complexes. The X-ray and NMR structure of protein-protein complex having a more flexible threshold of resolution are selected. For the dataset, if the calculated binding energy of analyzed protein interfaces is not appropriate (only the calculated energy within the range of \(-200—10\) kJ/mol is selected), the data are abandoned in analyses. Metal ions and water molecules are excluded in all analysis. The filtered set includes 654 “receptor

For each protein complex, the contributions of different interaction types to total binding energy are calculated by

\[ p_z = \frac{\sum A_{i,j} \times \Delta_{i,j}}{A} \]  

(4)

where \( z \) represents certain type of pair interaction (see Table 1). \( p_z \) is the energetic percentage of the interaction of type \( z \) to the total binding free energy of the calculated protein-protein complex. The pair interaction between atom \( i \) and \( j \) is the type \( z \), according to the definition in Table 1. The denominator \( A \) represents total PMF energy calculated by the equation 3.

4. Analysis of the stereochemistry of CH···O hydrogen bond

The stereochemical details of CH···O hydrogen bonds in some representative examples with a high energetic percentage of CH···O interactions were surveyed. Hydrogen atoms were added to these PDB coordinate files using CHARMM (61). Each of the CH···O hydrogen bond is analyzed using three different geometrical parameters: the C···O distance (d), H···O distance (dH) and C—H—O angle (θ). The definition of these parameters is shown in Table 2 and Table 3. In the analysis, only those contacts with a θ angle greater than 100° were accepted.

5. The comparisons of energy minimization calculations with and without the inclusion of the CH···O hydrogen bonding interaction energies

5.1 Model the CH···O=C weak hydrogen bond

We have modeled the CH···O=C weak hydrogen bond by adding a distance constraint:
and $k_{\text{min}}=200\text{kJ/(mol}^{\times}\text{Å}^{2})$, $k_{\text{max}}=100\text{kJ/(mol}^{\times}\text{Å}^{2})$, $r_{\text{min}}=3.2\text{Å}$, $r_{\text{max}}=3.4\text{Å}$.

Because we could not generate realistic binding energies using van der Waals interactions and partial charge electrostatics, a distance constraint is used to force $d(\text{C···O})$ to take on the observed value of $3.2\sim3.4\text{Å}$ in order to modeled the CH···O=C weak hydrogen bond. According to the potential shape of CH···O=C weak H-bond, two different force constants of the constraint are used in the close or long distance range respectively.

The resultant CH···O=C weak interaction potential is:

$$E_{\text{constraint}} = \begin{cases} 
0.5k_{\text{min}}(r_{\text{C}=\text{H}···\text{O}} - r_{\text{min}})^2 & r_{\text{C}=\text{H}···\text{O}} < r_{\text{min}} \\
0 & r_{\text{min}} < r_{\text{C}=\text{H}···\text{O}} < r_{\text{max}} \\
0.5k_{\text{max}}(r_{\text{C}=\text{H}···\text{O}} - r_{\text{max}})^2 & r_{\text{C}=\text{H}···\text{O}} > r_{\text{max}} 
\end{cases}$$

and the energetic terms of *van der Waals* interaction and electrostatic interaction are calculated by the values taken from CHARMM (60). The distance constraint is artificially stable and adequately simulates the *van der Waals* and partial interaction between the C and O atoms in the CH···O=C weak hydrogen bond.

**(2) Analysis of the stereochemistry of CH···O hydrogen bond based on the minimized structures with and without the inclusion of the CH····O hydrogen bonding interaction energies**

The crystal structures of the protein complexes were served as the starting point. The initial hydrogen atoms were added to these PDB coordinate files using CHARMM (60). Two different strategies are adopted during the minimization process of CHARMM. In the first one, the 2500 cycles of conjugate gradient minimizer (CONJ) is used until the energy convergence, and no atoms is fixed and the van der Waals interaction and electrostatic interaction are calculated as the nonbonded interaction of atom pair during the minimization process. In the other one, the 2500 cycles of conjugate gradient minimizer (CONJ) is also used until the energy convergence, and the distance constraint forcing the distance of C···O pair are added to the interaction energies in order to model
the CaH···O=C weak hydrogen bond. In all the minimization, the dielectric constant is simply set as 80 to simulate the water medium.

The first one is represented as the energy minimization calculation without the inclusion of the CH···O hydrogen bonding interaction energies, and the second one is represented as the energy minimization calculation with the inclusion of the CH···O hydrogen bonding interaction energies. The crystal structure is used as the reference structure for the purpose of comparisons. The C···O distances of the CH···O hydrogen bond in the different structures with and without the inclusion of the CH···O hydrogen bonding interaction energies are calculated, and the shift of C···O distance is analyzed.

[RESULT]

1. The Helmholtz free energy for general CH···O hydrogen bonding interactions

Based on the definition of the five atom types, the distance-dependent potentials are extracted from the training set. In Table 1 there are four atom pairs reflecting the type of CH···O pair interaction. We give emphasis to four atom pairs: A—CH, B—CH, CH—A and CH—B. In all cases, the occurrence of CH···O atom pair is sufficiently large: the number of CH-A(hydrogen bond acceptor) occurrence is 92026 and that of CH-B(both acceptor and donor) occurrence is 18101. Figure 1a and Figure 1b show the examples of the calculated Helmholtz free energy for these pair interactions, reflecting the characteristics of CH···O hydrogen bonding interactions. It is noted that the derived pair potentials for CH···O interaction have a favorable valley in the same distance range (~3.3Å) in all the figures, which matches well with those from quantum calculations (39).

Figure 1c shows the comparison of the calculated PMF energies of the three representative types of different interactions, including the D···A hydrogen bond as an example of conventional hydrogen bonds, the CH···A hydrogen bond, and the N···N non-polar pair interaction as an example of hydrophobic interactions. The calculated
energies of the three interactions have very different characterization: the example of conventional hydrogen bonding interactions has a favorable valley in the distance range from 2.4Å to 3.0Å and becomes weakly repulsive in the 3.3-4.2Å range; the example of CH···O hydrogen bonding interactions has a favorable valley in the distance range from 3.0Å to 3.5Å; and the example of hydrophobic interactions have a repulsive potential at all distances up to 4.5Å. The calculated energies of conventional hydrogen bond and CH···O hydrogen bond have different strength and optimum distance of maximum bonding strength: the conventional hydrogen bond has a bond strength of −5.5kJ/mol and an optimum distance of 2.8Å, while the CH···O hydrogen bond has a binding strength of −1.9kJ/mol and an optimum distance of 3.3Å. The CH···O hydrogen bond has a longer optimum distance and its strength is approximately one third of the conventional hydrogen bond.

2. Contribution of different interactions at protein-protein interfaces

Based on the new definition of five atom types, different interactions at protein interfaces can be classified easily. We have applied the potentials to the set of 469 protein-protein complexes. The Helmholtz free energies of different types of pair interactions at each protein interface were calculated and compared, including hydrophobic interactions, conventional hydrogen bonds and CH···O weak hydrogen bonds. And their energetic contributions were analyzed, focusing on their percentages in total energy of each calculated protein complex (using the equation 4). Then the mean value of every interaction percentages was calculated: The mean percentage of conventional hydrogen bonding interaction is around 30%, the mean percentage of hydrophobic interactions is 50%, and the mean contribution of CH···O interaction is 17%. In the Figure 2a the ratio of three interactions from the aspect of energetic contribution is shown. Furthermore we have analyzed the energetic percentage of CH···O hydrogen bonding interactions in each protein-protein complex. The distribution is shown in the Figure 2b.
It should be noted that the energetic percentages of CH···O hydrogen bonding interactions in some examples are up to 50% for protein-protein associations.

The steric interaction of atom types like hydrogen bond acceptor-acceptor and donor-donor is also analyzed with a mean percentage of 3%, which shows that it plays a weaker role at protein interfaces than the three major types of interactions (Figure 2b).

3. Structural features of CH···O interaction in some protein complexes with high CH···O interaction percentage

The protein-protein complexes with relatively high percentage of CH···O interaction have been analyzed (see Figure 2c). We carefully surveyed the geometrical parameters and structural features of these contacts in some representative examples, focusing on the contacts between adjacent β-strands and α-helices located at protein-protein interfaces.

3.1 Adjacent β-strands in parallel and anti-parallel orientations

In the representative examples with a high contribution of CH···O interaction, the stereochemistry of close CH···O contacts between adjacent β-strands at the interface has been analyzed. The PDB entries include 2kin, 2gac, 2bqp, 1pya, 1prt, 1lya, 1kvd, 1fi8, 1dgw and 1apy. Figure 2c shows the energetic percentage of CH···O interactions in each protein complex, which vary from 28.2% to 49.1%. In these representative examples, the CH···O contacts often occur between adjacent β-strands in parallel and anti-parallel orientations. The most common ones are the contacts involving α carbon and those involving main chain oxygen, especially the CαH···O=C(main chain) contact which occur frequently between adjacent strands at protein-protein interfaces. The detailed analysis of those CH···O contacts in all the representative examples is listed in the SUPPLEMENT materials.

Table 2 and Figure 3 show representative examples of CαH···O interactions between the β-strands of parallel and anti-parallel orientation and list their relevant stereochemical details. These stereochemical details are consistent with the geometry of the CαH···O
H-bond reported in different systems (17, 18, 58-60). There is an obvious structural feature in protein-protein interfaces: between adjacent $\beta$-strands in both parallel and anti-parallel orientations, the formation of the C$^\alpha$H···O H-bond combines with the conventional C=O···HN H-bond to form a bifurcated H-bond, where the carbonyl O atom on one strand forms a H-bond with both the amide H and the $\alpha$-carbon H atom on the other strand. Once the bifurcated H-bond is included, the adjacent $\beta$-strands of anti-parallel orientation (Figure 3b) looks remarkably like those of parallel orientation (Figure 3a).

3.2 Interhelical CH···O H-bonds in protein-protein interfaces

In the representative examples with a high contribution of CH···O interaction, the geometrical parameters of close CH···O contacts between adjacent $\alpha$-helices have been surveyed. The PDB entries including 2occ, 1wht, 1aig, 1ryp and 1qhg, have a high energetic percentage of CH···O interactions in each protein complex, varying from 28.8% to 44.2% (see Figure 2c). In these representative examples, the contacts involving polar side-chain carbon atoms frequently occur between adjacent $\alpha$-helices. Table 2 and Figure 4a show a representative example of CH···O interactions between anti-parallel $\alpha$-helices and list their relevant stereochemical details. The detailed analysis of those CH···O contacts is listed in the SUPPLEMENT materials.

The structural features and characterizations of close CH···O contacts between quasi-vertical helix segments are relatively few in number. Their structural features and characterizations are rather esoteric. So no further surveys were possible. Nevertheless it is still notable that these close CH···O interactions show the geometrical parameters very close to those of conventional hydrogen bonds (Table 2 and Figure 4b).

4. The comparisons of energy minimization calculations with and without the inclusion of the CH···O hydrogen bonding interaction energies
For the representative protein complex examples, the relevant stereochemical details of certain C\(^=\)H···O interactions between the \(\beta\)-strands of parallel and anti-parallel orientation are compared among the crystal structure and differently minimized structures with and without the inclusion of the CH···O hydrogen bonding interaction energies. Table 3 lists the C···O distances of the CH···O hydrogen bond between the adjacent \(\beta\)-strands in different structures. For the selected CH···O hydrogen bonds between adjacent \(\beta\)-strands in the two examples (2KIN and 1APY), the C···O distance shifts in the minimized structures are shown in figure 5a and figure 5b. It is clear that energy minimization without taking the CH···O hydrogen bonding into account will result larger C···O distances compared to the original crystal structures, which implies that the empirical force fields that treat CH···O contacts as repulsive needs to be modified for these examples.

[DISCUSSION]

1. The Simple atom type definition

Biological interfaces of protein-protein complexes contain many specific interactions, including hydrogen bonding, water bridging interactions, and nonspecific interactions (32, 33). In our method, the two atoms of each atom pair at protein-protein interfaces contact through either hydrogen bond (conventional or CH···O hydrogen bonding interactions) or hydrophobic interactions, which are pertinent on protein interfaces and tend to reflect the forces driving the association of protein complexes (see Table 1). In all the statistics, the occurrence of each the atom pair is sufficiently large. Moreover we omit the statistics in the distance shells having little atom pair occurrence to reduce the mistakes of insufficient statistics. We believe that the details of the potentials obtained are meaningful, which is the basis for the comparison of different interactions.
2. Is the CH···O pair interaction a real hydrogen bond?

As the favorable potential of CH···O interaction at protein-protein interfaces has not yet been obtained experimentally, we will discuss the question whether CH···O interaction is a real hydrogen bond or one of the nonspecific interactions based on the study here. The reasonable Helmholtz free energies of CH···O interaction at protein-protein interfaces are extracted using our method of mean-field potential. And the calculated energies obviously reflect the characterization of hydrogen bonding interaction. Recently the result of the ab initio quantum calculation shows that the binding energies of ideal CH···O pair interactions indicate the comparative hydrogen bond energy in the calculation between water molecules and some representative amino acids (39). Here using our statistical potentials from the training set of real protein-protein complexes, the calculated free energy has a reasonable potential form, which is similar to the quantum calculation of the ideal model.

At the same time, we find that the favorable valley of our calculated CH···O potential is very different from that of nonspecific interactions, which generally reflects the random contacts between atoms. In Figure 1c, the van der Waals repulsive potential of N···N atom pair is just one of the nonspecific interactions, which represents the distribution between non-bonded and randomly distributed non-polar atoms. These nonspecific interactions have an even potential close to zero at longer distances and have a rapidly climbing potential at short distances (up to 4.0Å). More importantly, they have no obviously favorable valleys at all distances. Thus the favorable valley of CH···O potential shows that different from random contacts, the CH···O pair interaction is one of the specific potentials, which has the characterization of hydrogen bonding interaction. Moreover, this shape of potential is similar to that of conventional hydrogen bond, in spite of the different strength and optimum distance. Thus the CH···O contact at protein-protein interfaces has specific interactions similar to conventional hydrogen bonds. According to the calculation of our PMF potential at protein-protein interfaces, the
CH···O contact should be considered as one of the hydrogen bonding interactions. Our conclusion is supported by the ab initio quantum calculation of Scheiner et al. (38, 39) that CH···O contacts appear to be a true hydrogen bond. Compared with the conventional hydrogen bond, the general CH···O hydrogen bond has rather weaker strength and longer optimum distance with its strength near one third of the conventional hydrogen bond and its optimum distance around 3.3Å.

3. The role of the three types of interactions at protein-protein interfaces: the quantitative calculation on energetic aspect

First we quantitatively calculate the energetic contribution of different types of interactions at protein-protein interfaces, which indicates the role of different forces at protein-protein interfaces. At the protein-protein interface, the average contribution of conventional hydrogen bond is around 30%; the percentage of CH···O hydrogen bond is around 17%; that of hydrophobic interaction is 50%; and the other steric interaction is 3%. Conventional hydrogen bonding and hydrophobic interactions are generally considered to play important roles in protein associations. The biggest contribution of hydrophobic interactions indicates that the large number of hydrophobic atom pairs occur at the protein-protein interface, because the energy of each hydrophobic atom pair is less than the other pair interactions. Also the 30% contribution of conventional hydrogen bonds shows the significant involvement of charged or polar residues in protein-protein association that is accepted widely (20, 21).

The most important finding here is that the energetic contribution of the CH···O weak hydrogen bonding interaction at protein-protein interfaces cannot be neglected. Close CH···O contacts abound at protein-protein interfaces. Although normally weaker than conventional hydrogen bonds, the number of CH···O contacts cannot be neglected. In our calculation of each protein-protein complex, it should be noted that the energetic
percentages of CH···O hydrogen bonding interactions in some examples are up to 30%–50% for protein-protein associations.

4. The structural features of CH···O hydrogen bonds at some protein interfaces with a high CH···O contribution: the bifurcated H-bond motif between adjacent β-strands

We have analyzed the protein-protein complexes with relatively high percentage of CH···O interactions, focusing on the geometrical parameters of the CH···O hydrogen bonds between adjacent β-strands and α-helices at the interface. These CH···O H-bonds appear to be a specific interaction favoring the formation and stabilization of the adjacent α-helices and β-strands (acting as a secondary hydrogen bond between β-strands compared with conventional C=O···HN hydrogen bond). Especially CαH···O H-bonds between adjacent strands in parallel and anti-parallel orientations have an important contribution at the protein interface. It is interesting to note that the structural motif of a bifurcated hydrogen bond is found between the adjacent strands at some representative examples of real protein interface (see Figure 3a and 3b). And the CH···O weak hydrogen bond secondarily effects the stabilization of the β-strands. In these examples, the CH···O interaction has a high energetic percentage of the total binding free energy, and the bifurcated H-bond motif appears to have an important contribution to the formation and stabilization of the parallel and anti-parallel β-strands.

In the protein complexes with strong CH···O interactions, close CαH···O contacts frequently occur between the parallel and anti-parallel β-strands, and the structural motif of bifurcated hydrogen bonds has been found between those adjacent strands. The CαH···O hydrogen bond is indispensable to form the bifurcated H-bond motif between β-strands. In these complexes, the CH···O hydrogen bonding interaction has a high percentage of binding free energy and thus plays an important role for the formation of the β-strands interactions at protein-protein interfaces.
5. Is the CH···O interaction important?

The quantitative PMF calculation of the energetic contribution has shown that the energetic contribution of the CH···O hydrogen bond has a mean value of 17% in the dataset of 469 protein complexes and cannot be neglected at protein-protein interfaces, which indicates the importance of the CH···O H-bond. Particularly it can be up to 30%~50% in some examples. In these examples, close CαH···O contacts often occur and the bifurcated H-bond motif commonly exists between parallel and anti-parallel β-strands at the interface, suggesting that they need to be paid more attention.

In fact, close CαH···O contacts often occur and the bifurcated H-bond motif commonly exists between parallel and anti-parallel β-strands in protein interiors and at protein-protein interfaces. There are many surveys of high-resolution protein structures that reveal the occurrence of CαH···O hydrogen bonds in both the parallel and anti-parallel β-sheets (18, 59). Very recently Ho & Curmi have reported that the twist and the shear of β-ribbon can be reproduced through the simulation of a simple model using bifurcated hydrogen bonds (60). In contrast, isolated β-strands are not twist in the molecular dynamics simulation where the CH···O=C pair is not considered as an H-bonded pair (62). This example shows that the CαH···O=C weak hydrogen bonds do have a strong impact on protein structures.

Our quantitative PMF calculation has shown the strong energetic contribution of the CH···O hydrogen bond between the β-strands in some examples. Furthermore, we have made comparisons of energy minimization calculations with and without the inclusion of the CH···O hydrogen bonding interaction energies. Our calculations have shown that the empirical force fields that treat CH···O contacts as non-H-bonded pair are not suitable in some examples, especially between adjacent β-strands.

Both Ho BK and Curmi PMG’s study and our own calculation suggest that that the CαH···O contact is a specific interaction favoring the formation of β-strands and the
bifurcated H-bond is an obvious structural feature between the adjacent β-strands, regardless of proteins or protein-protein interfaces. And they have an important contribution for the formation and stabilization of β-strands.

Moreover the observed geometrical parameters of all the close contacts are very close to those expected for hydrogen bonds. Recently stereochemical analysis of close CH···O contacts has reported that these contacts exhibit stereochemical features typical of hydrogen bonds in proteins, membrane proteins and active sites of proteases (17, 18, 58-60). Adding our observation at protein-protein interfaces, all of the studies show that CH···O H-bond appears to be a specific interaction having a favoring valley regardless of protein interiors, membrane proteins or protein-protein interfaces. However, those popular crystal refinement programs often treat the CH···O contact as a repulsive interaction. The importance of the CH···O interaction, indicated by our quantitative energetic calculation, calls for a revision of the refinement programs.

[CONCLUSION]

An empirical approach to quantitatively describe forces (including CH···O hydrogen bond) at protein interfaces in energetic aspect is presented here. Our calculated Helmholtz free energies of the CH···O pair have a similar favorite valley exhibiting the feature typical of hydrogen bond. When applying the scoring function to the set of protein-protein complexes, we found the significant contribution of CH·O hydrogen bonds. The average energetic contribution of the CH···O H-bond is 17% and this value in some complexes can reach as high as 40~50%. In these complexes, the structural motif of a bifurcated H-bond, combining the CαH···O H-bond with the conventional C=O···HN H-bond, is found between adjacent strands in both parallel and anti-parallel orientation at the interface.

In conclusion, the importance of CH···O hydrogen bonding interactions calls for a revision for the point of view that CH···O contacts are treated as repulsive. When
studying protein-protein interfaces, the CH···O type hydrogen bonds should be taken into appropriate consideration.

[Acknowledgement]

We thank Dr. Chao Tang for inspiring discussions of the simple model of CH···O type hydrogen bonds, Ying Gao for kindly supplying the data set, Hao Chen for helpful assistance in energy minimization, and all the other members of the Lai group for helpful discussions. This work has been supported by the National Natural Science Foundation of China (No.29525306, No.20173001), the Ministry of Science and Technology of China, and the Commission of Science and Technology of Beijing.

[REFERENCES]


Figure Legends

Figure 1. The potentials of mean force for CH···O pair interactions using five atom types
In all figures the dots are merely connected by smooth curves for visualization and no smoothing procedure is used. As there are less than 30 observations in the distance range of 0—2.4Å, the figure is short of statistics in that distance range. In order to reflect the trends of the potentials in the range, the broken line is appended.
Figure 1a. The potentials for the hydrogen bond acceptor-CH type interactions (A-CH and CH-A) in protein-protein associations are shown. The black curve represents the A-CH interaction and the red curve represents the CH-A interaction.
Figure 1b. The potentials for type N and type CH interactions (B-CH and CH-B) in protein-protein associations are shown. The black curve is the B-CH interaction and the red curve is the CH-B interaction.
Figure 1c. The potentials for the three representative types of different interactions are shown. The black curve is the D-A hydrogen bonding interaction, the red curve is the CH--O H-bonding interaction and the green one is the non-polar pair interaction between atoms of type N.

Figure 2. The contribution of CH···O hydrogen bonding interactions in protein-protein complexes
Figure 2a. The average contribution of conventional hydrogen bonding interactions, hydrophobic interactions, and CH···O interactions
Figure 2b. The distribution of the percentages of CH···O hydrogen bonding interactions in total binding energy of protein-protein complexes is shown. Y-axis represents the number of occurrence.

Figure 2c. The examples of protein complexes with strong contribution of CH···O interactions are shown. X-axis represents the CH···O interaction percentage in the protein-protein complex. The protein-protein complexes are denoted by PDB codes.

Figure 3. The representative examples of CαH···O contacts between adjacent β-strands
Purple lines show conventional NH···O=C hydrogen bonds, and green lines indicate the CαH···O contacts. Only main-chain atoms are shown with the conventional color codes: oxygen-red, nitrogen-blue, carbon-black, and hydrogen-white.

Figure 3a. A representative example of CαH···O contacts between adjacent strands of a parallel orientation in the kinesin dimer (2KIN) is shown. The displayed atoms are at the interface between the chain A and chain B of the dimer.

Figure 3b. A representative example of CαH···O contacts between adjacent strands of an anti-parallel orientation in the human aspartylglucosaminidase (1APY) is shown. The displayed atoms are at the interface between the chain A and chain B of the heterotetrameric structure of the human aspartylglucosaminidase.

Figure 4. The representative examples of CH···O contacts between adjacent α-helices
Figure 4a. A representative example of CH···O contacts between adjacent helices of an anti-parallel orientation in the serine carboxypeptidase complex (1WHT) is shown. The displayed atoms are at the interface between the chain A and chain B of the complex. For other details refer to Figure 3.
Figure 4b. A representative example of CH···O contacts adjacent α-helices of a quasi-vertical orientation in the yeast proteasome (1RYP) is shown. The analyzed interface is between the chain K and chain Z of the multi-chain proteinase. For other details refer to Figure 3.

Figure 5. The comparisons of the C···O distances of the C$^a$H···O contacts between adjacent β-strands with and without the inclusion of the CH···O hydrogen bonding interaction energies

The Y axle is represented as the shift of the C···O distance of the minimized structure compared with crystal structure. Red column shows the shift of the C···O distance of the minimized structure without the inclusion of the CH···O hydrogen bonding interaction energies, compared with that in the crystal structure. And green column shows the shift of the C···O distance of the minimized structure with the inclusion of the CH···O hydrogen bonding interaction energies, compared with that in the crystal structure.

Figure 5a. The shift of the C···O distance of C$^a$H···O contacts between adjacent strands of a parallel orientation in the kinesin dimer (2KIN) is shown.

Figure 5b. The shift of the C···O distance of C$^a$H···O contacts between adjacent strands of an anti-parallel orientation in the human aspartylglucosaminidase (1APY) is shown.
Table 1. Atom pairwise interaction types

<table>
<thead>
<tr>
<th>Atom type</th>
<th>A&lt;sup&gt;a&lt;/sup&gt;</th>
<th>D&lt;sup&gt;b&lt;/sup&gt;</th>
<th>CH&lt;sup&gt;c&lt;/sup&gt;</th>
<th>N&lt;sup&gt;d&lt;/sup&gt;</th>
<th>B&lt;sup&gt;e&lt;/sup&gt;</th>
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<tbody>
<tr>
<td>A</td>
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<td>conventional hydrogen bond</td>
<td>CH···O hydrogen bond</td>
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<td>conventional hydrogen bond</td>
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<tr>
<td>a. hydrogen bond acceptor</td>
<td>b. hydrogen bond donor</td>
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<td></td>
<td></td>
<td></td>
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<tr>
<td>D</td>
<td>conventional hydrogen bond</td>
<td>━</td>
<td>hydrophobic</td>
<td>hydrophobic</td>
<td>conventional hydrogen bond</td>
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<td>CH</td>
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<td>hydrophobic</td>
<td>hydrophobic</td>
<td>hydrophobic</td>
<td>hydrophobic</td>
</tr>
<tr>
<td>B</td>
<td>conventional hydrogen bond</td>
<td>conventional hydrogen bond</td>
<td>CH···O hydrogen bond</td>
<td>hydrophobic</td>
<td>conventional hydrogen bond</td>
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<tr>
<td>e. both hydrogen bond donor and acceptor</td>
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<tr>
<td>f. steric interaction.</td>
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Table 2. The stereochemistry of selected CH···O hydrogen bonds in some representative examples.

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<th>C-H donor</th>
<th>Calculated energy(^a) (kJ/mol)</th>
<th>(d) (Å)</th>
<th>(d_{ll}) (Å)</th>
<th>(\theta) (°)</th>
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<tr>
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<td>O 297(^b)Arg</td>
<td>C(^a) 80(^b)Gly</td>
<td>-1.9</td>
<td>3.22</td>
<td>2.26</td>
<td>145.6</td>
</tr>
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<td>2KIN</td>
<td>O 81(^b)Thr</td>
<td>C(^a) 298(^b)Thr</td>
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<td>2KIN</td>
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<td>C(^a) 82(^b)Ile</td>
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<td>C(^a) 300(^b)Ile</td>
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<td>C(^a) 84(^b)Ala</td>
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<td>3.22</td>
<td>2.26</td>
<td>145.9</td>
</tr>
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<td>2KIN</td>
<td>O 85(^b)Tyr</td>
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<tr>
<td>1APY</td>
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<td>C(^a) 200(^b)Ser</td>
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<td>C(^a) 66(^b)Ala</td>
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<td>C(^a) 198(^b)Gly</td>
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<td>C(^a) 196(^b)Ala</td>
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<td>2.40</td>
<td>132.5</td>
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<td>3.29</td>
<td>2.31</td>
<td>146.4</td>
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</table>

a. the pair energy is re-calculated by the potentials  
b. the interatomic C···O distance (d), representing the donor-accepter distance of the CH···O hydrogen bond
c. \( d_H \) represents the H\( \cdots \)O distance, i.e. CH\( \cdots \)O H-bond distance

d. \( \theta \) represents the C—H—O angle of the CH\( \cdots \)O hydrogen bond

Table 3. The comparisons of energy minimization calculations with and without the inclusion of the CH\( \cdots \)O hydrogen bonding interaction energies

<table>
<thead>
<tr>
<th>PDB entry</th>
<th>Acceptor</th>
<th>C-H donor</th>
<th>( d_0 ) (Å)</th>
<th>( d' ) (Å)</th>
<th>( d'' ) (Å)</th>
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<td><strong>adjacent ( \beta )-strands in parallel orientation</strong></td>
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</tr>
<tr>
<td>2KIN</td>
<td>O 297( ^\beta )Arg</td>
<td>C( ^a ) 80( ^\alpha )Gly</td>
<td>3.22</td>
<td>3.52</td>
<td>3.37</td>
</tr>
<tr>
<td>2KIN</td>
<td>O 81( ^\alpha )Thr</td>
<td>C( ^a ) 298( ^\beta )Thr</td>
<td>3.44</td>
<td>3.71</td>
<td>3.40</td>
</tr>
<tr>
<td>2KIN</td>
<td>O 299( ^\beta )Thr</td>
<td>C( ^a ) 82( ^\alpha )Ile</td>
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<td>2KIN</td>
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<td>O 301( ^\beta )Val</td>
<td>C( ^a ) 84( ^\alpha )Ala</td>
<td>3.22</td>
<td>3.39</td>
<td>3.24</td>
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<tr>
<td>2KIN</td>
<td>O 85( ^\alpha )Tyr</td>
<td>C( ^a ) 302( ^\beta )Ile</td>
<td>3.29</td>
<td>3.57</td>
<td>3.32</td>
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<td><strong>adjacent ( \beta )-strands in anti-parallel orientation</strong></td>
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<tr>
<td>1APY</td>
<td>O 65( ^\alpha )Asp</td>
<td>C( ^a ) 200( ^\beta )Ser</td>
<td>3.53</td>
<td>3.57</td>
<td>3.42</td>
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<tr>
<td>1APY</td>
<td>O 199( ^\beta )Thr</td>
<td>C( ^a ) 66( ^\alpha )Ala</td>
<td>3.40</td>
<td>3.56</td>
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<td>1APY</td>
<td>O 67( ^\alpha )Met</td>
<td>C( ^a ) 198( ^\beta )Gly</td>
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<td>3.29</td>
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<td>1APY</td>
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<tr>
<td>1APY</td>
<td>O 69( ^\alpha )Met</td>
<td>C( ^a ) 196( ^\beta )Ala</td>
<td>3.23</td>
<td>3.29</td>
<td>3.25</td>
</tr>
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</table>

a. the interatomic C\( \cdots \)O distance (d) in the crystal structure
b. the interatomic C\( \cdots \)O distance (d') in the minimized structure without the inclusion of the CH\( \cdots \)O hydrogen bonding interaction energies
c. the interatomic C\( \cdots \)O distance (d'') in the minimized structure with the inclusion of the CH\( \cdots \)O hydrogen bonding interaction energies
**Figure 1a** Jiang L. et.al.

![Figure 1a](image)

**Calculated energy (kJ/mol)**

**Distance (angstrom)**

**Figure 1b** Jiang L. et.al.

![Figure 1b](image)

**Calculated energy (KJ/mol)**

**Distance (angstrom)**
Figure 1c Jiang L. et.al.
Figure 2a Jiang L. et.al.

Figure 2b Jiang L. et.al.
Figure 2c Jiang L. et.al.

![Energetic percentage chart from Figure 2c](image-url)
Figure 4a. Jiang L. et al.

Figure 4b. Jiang L. et al.
Figure 5a Jiang L. et al.

[Graph showing data for 2KIN with red bars indicating 'without the inclusion of the CH...O energies' and green bars indicating 'with the inclusion of the CH...O energies'.]

Figure 5b Jiang L. et al.

[Graph showing data for 1APY with red bars indicating 'without the inclusion of the CH...O energies' and green bars indicating 'with the inclusion of the CH...O energies'.]
Corresponding Author:

Luhua Lai

Institute of Physical Chemistry, College of Chemistry and Molecular Engineering & State Key Laboratory for Structural Chemistry of Unstable and Stable Species

Peking University

Beijing, 100871

P. R. China

Tel: 86-10-62757486; Fax: 86-10-62751725

E-mail: lhlai@pku.edu.cn or lai@mdl.ipc.pku.edu.cn
The larger set of 469 protein complexes (including 654 “receptor protein-ligand complex” pairs)
The detailed analysis of CH...O contacts in protein-protein complexes having a high CH...O contribution

1. CH...O contacts between parallel β-strands in some protein complexes

<table>
<thead>
<tr>
<th>Res1</th>
<th>Res2</th>
<th>Dist (Å)</th>
<th>Type</th>
<th>Atom1</th>
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<tbody>
<tr>
<td>LYS10</td>
<td>THR299</td>
<td>3.325</td>
<td>O</td>
<td>LYS A 10 CA</td>
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<td>VAL11</td>
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<td>MET12</td>
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<td>CY515</td>
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<td>CY5 A 15 O</td>
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2. CH...O contacts between antiparallel β-strands

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3. CH...O contacts between antiparallel β-strands

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| TRP29        | ASP132   | 3.101  | 14   | O     | THR A    | 29     | CA  | ASP B |
| ASN29        | ASP132   | 3.301  | 14   | O     | THR A    | 29     | CB  | ASP B |
| THR29        | PHE131   | 3.473  | 34   | OG1   | THR A    | 29     | CA  | PHE B |
| VAL51        | GLY135   | 3.104  | 41   | CA    | VAL A    | 30     | O    | GLY B |
| VAL51        | GLY135   | 3.368  | 41   | CB    | VAL A    | 30     | O    | GLY B |
| VAL51        | ILE134   | 3.654  | 14   | O     | VAL A    | 31     | CA   | ILE B |
| PHE52        | LEU135   | 3.372  | 41   | CA    | PHE A    | 32     | O    | LEU B |
| ASP53        | GLY136   | 3.259  | 14   | O     | ASP A    | 33     | CA   | GLY B |

| Select       | LEE19    | 3.367  | 14   | O     | LEE A    | 59     | CA  | PHE B |
| LEE19        | PHE115   | 3.145  | 14   | O     | LEE A    | 59     | CB  | PHE B |
| TRP10        | GLY116   | 3.251  | 41   | CA    | TRP A    | 40     | O    | GLY B |
| TRP10        | GLY116   | 3.400  | 41   | CB    | TRP A    | 40     | O    | GLY B |
| VAL41        | GLU117   | 3.661  | 14   | O     | VAL A    | 41     | CA  | GLU B |
| VAL41        | ALA110   | 3.307  | 14   | O     | VAL A    | 41     | CB  | ALA B |
| SER15        | ALA110   | 3.611  | 41   | CA    | SER A    | 43     | O    | ALA B |
| SER15        | ALA110   | 3.209  | 41   | CB    | SER A    | 43     | O    | ALA B |

| Select       | ILE127   | 3.420  | 41   | CD1   | ILE A    | 55     | O    | ILE B |
| GLY85        | THR119   | 3.218  | 43   | CA    | GLY A    | 85     | OG1 | THR B |

**lkvd_A_B anti-parallel B-strands**

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| LEE21        | THR119   | 3.604  | 41   | CA    | LEE A    | 21     | O    | THR B |
| ARG22        | SER191   | 3.157  | 14   | O     | ARG A    | 22     | CA  | SER B |
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| MET25        | VAL168   | 3.358  | 41   | CA    | MET A    | 25     | O    | VAL B |
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| GLN26        | VAL168   | 3.577  | 41   | CB    | GLN A    | 26     | O    | VAL B |
| LYS27        | GLY167   | 3.116  | 14   | LYS A  | 27     | CA   | GLY B |

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2. CH...O contacts between parallel α-helices in some protein complexes

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| select | ASP25 | ARG43 # 3.595 | 14 | OD2 | ASP_B | 25 CD | ARG_I | 43 |
| select | GLU26 | TYR35 # 3.634 | 14 | CD2 | LEU_B | 28 OH | TYR_I | 55 |

1whl_A_B anti-parallel α-helices

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| select | GLU47 | THR271 # 3.530 | 14 | OE1 | GLU_A | 64 CB | THR_B | 271 |
| select | GLU47 | LEU401 # 3.774 | 14 | O | GLU_A | 64 CA | LEU_B | 401 |
| select | GLU47 | LEU401 # 3.196 | 14 | O | GLU_A | 64 CB | LEU_B | 401 |
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| select | HIS133 | SER349 # 3.308 | 14 | CB | HIS_A | 183 OG | SER_B | 349 |
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| select | ASP104 | ALA345 # 3.417 | 14 | O | ASP_A | 181 CB | ALA_B | 345 |
| select | ASP104 | ALA345 # 3.709 | 14 | OD1 | ASP_A | 181 CB | ALA_B | 345 |
| select | GLY107 | THR344 # 3.849 | 14 | CA | GLY_A | 187 O | THR_B | 344 |
| select | GLY107 | THR344 # 3.411 | 14 | O | GLY_A | 187 CB | THR_B | 344 |

laig_N_O anti-parallel α-helices

| select | LYS8 | GLU246 # 3.557 | 14 | CE | LYS_N | 8 OE1 | GLU_O | 246 |
| select | TYR9 | GLU246 # 3.524 | 14 | OH | TYR_N | 9 CB | GLU_O | 246 |
| select | ILE107 | THR253 # 3.193 | 14 | CD1 | ILE_N | 107 OG1 | THR_O | 255 |
| select | LEU111 | ARG243 # 3.179 | 14 | O | LEU_N | 111 CD | ARG_O | 247 |
### 5. CH...O contacts between quasi-vertical α-helices in protein complex

<table>
<thead>
<tr>
<th>Res1</th>
<th>Res2</th>
<th>Dist (Å)</th>
<th>Type</th>
<th>Atom1</th>
<th>Atom2</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Lys_K</strong> quasi-vertical α-helices</td>
<td></td>
<td></td>
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<tr>
<td>select PHE157</td>
<td>THR154</td>
<td>3.111</td>
<td>0</td>
<td>PHE K 137 CB</td>
<td>THR Z 154</td>
</tr>
<tr>
<td>select PHE157</td>
<td>THR154</td>
<td>3.116</td>
<td>43</td>
<td>CB PHE K 137 OG1</td>
<td>THR Z 154</td>
</tr>
<tr>
<td>select SER141</td>
<td>PHE155</td>
<td>3.260</td>
<td>41</td>
<td>CB SER K 141 O</td>
<td>PHE Z 155</td>
</tr>
<tr>
<td>select SER141</td>
<td>GLY158</td>
<td>3.695</td>
<td>34</td>
<td>OG SER K 141 CA</td>
<td>GLY Z 158</td>
</tr>
<tr>
<td>select GLU166</td>
<td>TYR157</td>
<td>3.661</td>
<td>14</td>
<td>OE2 GLU K 166 CB</td>
<td>TYR Z 157</td>
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<tr>
<td>select GLU166</td>
<td>GLY158</td>
<td>3.634</td>
<td>14</td>
<td>OE2 GLU K 166 CA</td>
<td>GLY Z 158</td>
</tr>
<tr>
<td>select ASP141</td>
<td>ASP141</td>
<td>3.283</td>
<td>41</td>
<td>OE1 ASP K 141 CB</td>
<td>ASP Z 141</td>
</tr>
<tr>
<td>select LYS169</td>
<td>ASP141</td>
<td>3.283</td>
<td>41</td>
<td>CD LYS K 169 OD2</td>
<td>ASP Z 141</td>
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<td><strong>Lys_A_H</strong> quasi-vertical α-helices</td>
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<tr>
<td>select LEE49</td>
<td>GLN49</td>
<td>3.226</td>
<td>41</td>
<td>CD1 LEU A 155 OE1 GLN H 69</td>
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<tr>
<td>select LYS590</td>
<td>SER488</td>
<td>3.328</td>
<td>41</td>
<td>CE LYS A 388 O</td>
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<tr>
<td>select ARG1013</td>
<td>GLU64</td>
<td>3.145</td>
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<td>CB ARG A 1015 OE2 GLU H 64</td>
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<td><strong>Lys_2_1</strong> quasi-vertical α-helices</td>
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<tr>
<td>select MET142</td>
<td>ALA36</td>
<td>3.107</td>
<td>14</td>
<td>O MET 2 142 CB</td>
<td>ALA 1 136</td>
</tr>
<tr>
<td>select MET142</td>
<td>LEE132</td>
<td>3.539</td>
<td>43</td>
<td>CE MET 2 142 O</td>
<td>LEU 1 132</td>
</tr>
<tr>
<td>select LEE146</td>
<td>SER140</td>
<td>3.535</td>
<td>43</td>
<td>CD1 LEU 2 146 OG</td>
<td>SER 1 114</td>
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<tr>
<td>select LEE146</td>
<td>ALA36</td>
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<td>CD2 LEU 2 146 O</td>
<td>ALA 1 136</td>
</tr>
<tr>
<td>select LEE146</td>
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<td>3.157</td>
<td>43</td>
<td>CD2 LEU 2 146 OG</td>
<td>SER 1 114</td>
</tr>
<tr>
<td>select PRO115</td>
<td>ASN163</td>
<td>3.591</td>
<td>41</td>
<td>CA PRO 2 145 OD1</td>
<td>ASN 1 165</td>
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<tr>
<td>select PRO115</td>
<td>ASN163</td>
<td>3.103</td>
<td>41</td>
<td>CB PRO 2 145 OD1</td>
<td>ASN 1 165</td>
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</tbody>
</table>
select ARG179 || GLU139 # 3.151 41 CD ARG 2 179 O2E GLU 1 139

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lqkg_B_C quasi-vertical α-helices

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select ARG365 || GLU518 # 3.291 41 CD ARG B 365 O2E GLU C 518

select GLU591 || ARG508 # 3.414 14 OE1 GLU B 591 CD ARG C 508
select GLU591 || ASN511 # 3.503 14 OE2 GLU B 591 CB ASN C 511
select ILE592 || ASN511 # 3.528 41 CD1 ILE B 592 O ASN C 511

select LEU599 || LEU599 # 3.503 14 O LEU B 599 CD1 LEU C 551
select VAL401 || LEU468 # 3.659 14 O VAL B 401 CD2 LEU C 468
CH...O hydrogen bonds at protein-protein interfaces
Lin Jiang and Luhua Lai

J. Biol. Chem. published online July 15, 2002

Access the most updated version of this article at doi: 10.1074/jbc.M204514200

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