Table 5. *Peaks near model solvent positions in 'imaginary' Fourier map using sulfur-as-sulfur model for phases*

	Peak-to-atom distance (Å)	Rank*	Peak height, σ†
Azil38N2	0·51	25	3·2
Azil46N2	0·86	38	3·0
Wat2030	0·83	56	2·9
Wat2810	0·97	32	3·2

* Ranking excludes ripples due to the iron atoms.

† Peak heights are measured in units of standard deviations where σ is the r.m.s. density of the map.

very unequal. Since the electron density at these positions was fairly linear, we decided to substitute azide for sulfate at these solvent sites. However, when we searched either 'imaginary' or Kraut Bijvoet-difference Fourier maps for peaks corresponding to solvent atoms, only four peaks met the criteria of being within 1·0 Å of a solvent site and having a peak height of at least 2·75 times the r.m.s. density. The two sulfate positions were among these (Table 5). The third position, which was the weakest, was about 3·1 Å from one of the two sulfates and did not correspond to any density that could be attributed to a sulfate. The fourth position was the farthest from a solvent site. This site had been modeled as an 'either/or' disordered site with another water, but it was so weak that it was removed from the model at a later stage. On the basis of these results we have returned to our interpretation of two positions as sulfate anions.

In conclusion we find the 'imaginary' Fourier to be very useful when the information is available for its calculation. However, one must be cautious about interpreting such maps due to the considerable bias in the phases (Hendrickson & Sheriff, 1987). Without this bias, the 'imaginary' Fourier is still better than the Kraut Bijvoet-difference Fourier, largely because the noise level is below that of the Kraut function.

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Peptide Chain Structure Parameters, Bond Angles and Conformational Angles from the Cambridge Structural Database

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Abstract

An analysis of the bond angles and conformational angles in the oligopeptide crystals accumulated in the Cambridge Structural Database has been carried out to obtain precise information essential to protein structural studies. The peptide torsion angles ω distribute asymmetrically around 157-201°; $\omega < 170°$ occurs with probability 7%, but $\omega > 190°$ less than 3%. The $\tau(C^{\alpha}C'N)$ and $\tau(C'NC^{\alpha})$ angles do not depend on the structures of the main and side chains. But the $\tau(NC^{\alpha}C')$ angles depend on ψ as well as the side-chain shapes, being in the wide range 103-117°. For each amino-acid residue the mean $\tau(NC^{\alpha}C')$ angle in the folded-chain region with $\psi = -50$-30° is about 4° larger than that in the extended-chain region with $\psi = 100$-210°; in the same ψ region the angle of Gly is the largest and that of Val, Ile and Thr is the smallest, their difference being about 3°. The side-chain conformations of $(N^{\alpha}-C^{\alpha}-C^{\beta}-C^{\gamma})$ are strongly

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constrained to the *gauche* or *trans* forms: the maximum deviation of χ^1 from the ideal angles is only 27°, and the eclipsed conformations with χ^1 close to 0 or ±120° are not found.

Introduction

The structure analyses of amino acids and peptides have provided much reliable information and precise parameters, such as bond angles and conformational angles, which are indispensable for the structural studies of proteins. They are particularly of significance for the refinement of protein crystal structures at low resolution insufficient for atomic resolution, theoretical structural studies of proteins by model building, drug design, protein engineering *etc.*

In this decade many accurate structure analyses of oligopeptide crystals have been carried out, and their structural data have been accumulated in the Cambridge Structural Database (CSD; Allen, Bellard, Brice, Cartwright, Doubleday, Higgs, Hummelink, Hummelink-Peters, Kennard, Motherwell, Rodgers & Watson, 1979). The present study involves an analysis of the structural data, especially bond angles and conformational angles of the peptide main chain and the side-chain conformations, of the peptides in CSD. Some results seem to be of essential importance for protein structural studies.

The database in this University in May 1985 contained 1139 entries in class 48, α-amino acids and peptides. Among these the structural data of 325 unique crystals were available for this study, which include 161 linear oligopeptides, 29 cyclic peptides with five to ten residues, 39 amino acids having at least one peptide bond made with groups such as acetyl, alkylamide *etc.*, 88 amino acids (monomers) and 8 depsipeptides. The small cyclic peptides of two, three and four residues (31 crystals) were used only for the study of side-chain conformations, because severe strains may be present in the main-chain structures due to the small-ring formation. The crystal structures determined with *R* factors larger than 10% were omitted from this study because of the inaccuracies in their structural parameters. The bond angles and conformational angles were estimated from CSD by the program *GEOM*78 in its retrieval system.*

The three-letter symbols are used for the 20 common amino acids. The abbreviations are: Xxx: any L-α-amino-acid residues including non-common amino acids and the groups such as acetyl- and -*N*-alkylamide; nonPro: any amino-acid residue except Pro and Hyp; Aib: α-amino isobutyric acid; nonGly: any α-amino-acid residues except Gly, Pro and Hyp. $\tau(C^\alpha)$, $\tau(C')$ and $\tau(N)$ stand for the bond angles $\tau(NC^\alpha C')$, $\tau(C^\alpha C'N)$ and $\tau(C'NC^\alpha)$, respectively. The internal rotation angle of N^α–C^α–C^β–C^γ is denoted by χ^1. The notations of atoms and the conformational angles of the main and side chains are those defined by the IUPAC-IUB Commission on Biochemical Nomenclature (1970).

The peptide bond

476 peptide bonds were available to this study. They are divided into three groups based on the structure characteristics, that is 393 (*trans*) Xxx-nonPro peptide bonds, 68 *trans* Xxx-Pro bonds, and 15 *cis* Xxx-Pro bonds.

Torsion angle ω

The distribution of ω of the *trans* form is shown in Fig. 1. The mean values, e.s.d.'s and the minimum and maximum values of ω's in the three groups are:

trans Xxx-nonPro	178·9 (64)°	157–201°
trans Xxx-Pro	179·7 (51)°	169–190°
cis Xxx-Pro	0·9 (104)°	−19–20°

In many peptide bonds the torsion angle ω shows large deviations from the ideal value of 180°; a deviation of more than 10° from planarity is not unusual, occurring with a probability of about 10%. Even a large deviation of about 20° is occasionally possible. A deviation of ω of about 12° corresponds to a potential-energy increase of 4·2 kJ mol^{-1} (Schultz & Schirmer, 1979). The distribution of ω about its mean value is neither normal nor symmetrical. ω is in the range 160–170° at a probability of about 7%, in contrast to <3% for the range −160 to −170°. Such an asymmetric deviation of ω from 180° is certainly a consequence of the asymmetric disposition of atoms around the peptide linkages. Similar distributions of ω, in both asymmetry and magnitudes, have been reported, for instance, in elastase (Sawyer, Shotton, Campbell, Wendell, Muirhead & Watson, 1978) and bovine pancreatic trypsin inhibitor (Deisenhofer & Steigemann, 1975).

The ω angles in the *trans* Xxx-Pro bonds are distributed in the range 169–190°, and the deviations from planarity are rather smaller than those in the usual Xxx-nonPro bonds between the common amino acids.

Bond angles τ(C′) and τ(N)

The bond angles for the three groups of peptide bonds are shown in Fig. 2. Those for the Xxx-nonPro bonds especially are sharply and normally distributed

* Lists of CSD reference codes for the peptide crystals, ω, $\tau(C')$ and $\tau(N)$ of the peptide bonds, and $\tau(C^\alpha)$, φ, ψ, χ's of the amino-acid residues have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43378 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

around their mean values, showing that the two bond angles do not significantly depend on the conformations of the main chain and/or the side chain. Their mean values, e.s.d.'s and the minimum and maximum values in the data are:

trans Xxx-nonPro	τ(C′)	116·2 (21)°	110–125°
	τ(N)	121·5 (18)°	115–126°
trans Xxx-Pro	τ(C′)	117·2 (17)°	112–121°
	τ(N)	119·9 (11)°	117–123°
cis Xxx-Pro	τ(C′)	118·0 (17)°	115–121°
	τ(N)	126·1 (13)°	124–129°

As reported earlier, τ(C′) in the *trans* Xxx-Pro bonds is larger than that in the *trans* Xxx-nonPro bonds, because of the presence of a bulky C^{δ} methylene group of the pyrrolidine ring (Ashida & Kakudo, 1974). The $C^{\delta}NC^{\alpha}$ angle of the pyrrolidine ring in the oligopeptides is 114°, and the $C'NC^{\delta}$ angle is 126° in *trans* Xxx-Pro and 120° in *cis* Xxx-Pro (Ashida, Tanaka, Yamane & Kakudo, 1978).

(φ, ψ) plot

The Ramachandran plot of (φ, ψ) of 462 residues for which both N and C′ participate in peptide bonds is shown in Fig. 3. Some features of the plot are different from those of many globular proteins, mainly because the relative frequency of the secondary structures in the oligopeptides is different from that in globular proteins.

Most of the residues having $\varphi > 0°$ are Gly except for a few residues involved in the left-handed α helices, which are found in peptides containing the uncommon amino acid Aib. Besides, very few residues in the peptides containing Aib have $\varphi < 0°$ for the right-handed α helix or the 3_{10} helix. The right-handed α helix of more than one turn made solely of the common amino acids has not yet been reported.

The type I β turn is the secondary structure which is most frequently found in the oligopeptide crystals (Ashida, Tanaka, Yamane & Kakudo, 1978). Many linear oligopeptides, and most of the cyclic oligopeptides consisting of more than five residues have a β turn, mostly of type I. In the Ramachandran plots of many globular proteins as well as the present one for the oligopeptides, many (φ, ψ) dots around (−90°, 0°)

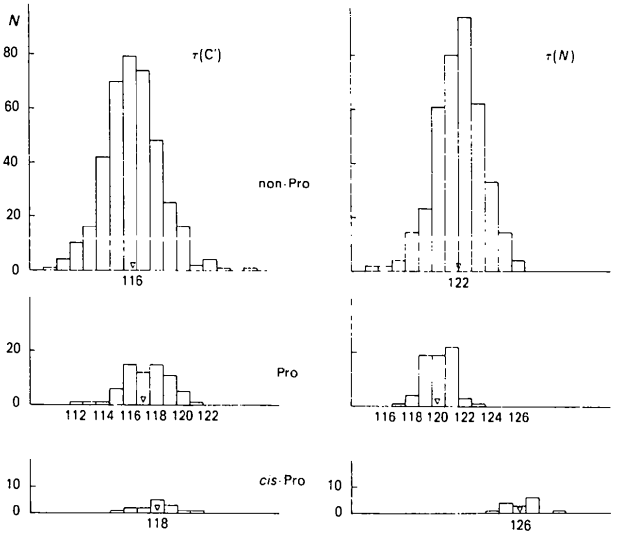

Fig. 2. τ(C′) and τ(N) in the peptide bonds of *trans* Xxx-nonPro, *trans* Xxx-Pro and *cis* Xxx-Pro.

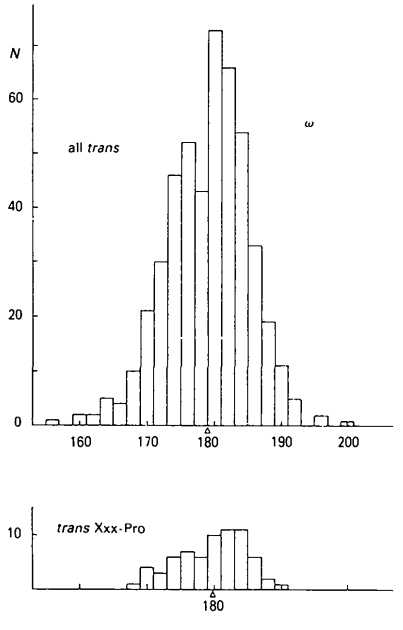

Fig. 1. Histograms of ω in all the *trans* peptide bonds and the *trans* Xxx-Pro bonds. The mean angles are shown by small triangles.

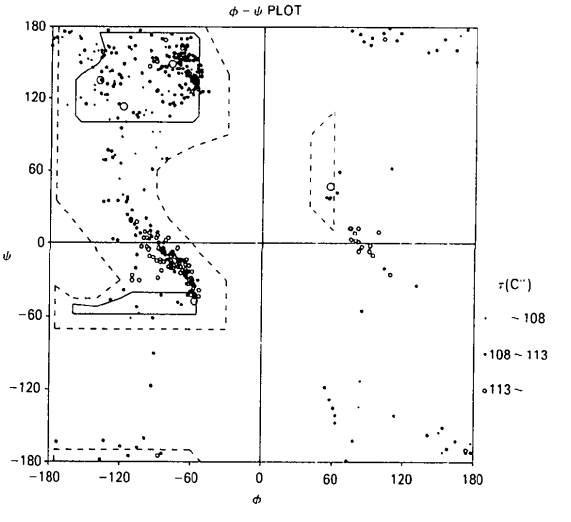

Fig. 3. Ramachandran plot of (φ, ψ) of all the residues. The size of the spots roughly shows magnitudes of $\tau(C^{\alpha})$. The large open circles show the torsion angles of the secondary structures.

correspond to the type I β turn. This region is called the 'bridge region' since it connects the extended-chain region and the helix region (Schultz & Schirmer, 1979). Most of the dots in this region gather around the line $\psi = -\varphi - 90$, because of the negative correlation between φ and ψ for the type I β turn (Tanaka, Ashida, Shimonishi & Kakudo, 1979). The β turn of type II also is often found in the oligopeptides. A cluster of dots around $(-60°, 135°)$ in the extended-chain region corresponds to the second residues in the type II β turn, and several Gly residues around $(90°, 0°)$ are those of the third residues. There are also a few β turns of type I′ and II′.

Many residues, mostly Pro, having conformations similar to that of the poly(L-proline) II helix or in collagen are found around $(-66 \pm 11°, 152 \pm 14°)$, which are the mean torsion angles of Pro in several peptides having a poly(L-proline) II helix. These mean torsion angles deviate significantly from $(-78°, 149°)$ given by Arnott & Dover (1968) for the poly(L-proline) II helix.

Bond angle $\tau(C^\alpha)$

It is well known that $\tau(C^\alpha)$ sometimes deviates significantly from the mean (standard) value of 111° given by Marsh & Donohue (1967). For instance, the mean $\tau(C^\alpha)$ angles are 111·5° in tosyl-α-chymotrypsin (Birktoft & Blow, 1972), 112·7° in elastase (Sawyer *et al.*, 1978) and 111·8 (58)° in bovine pancreatic trypsin inhibitor (Deisenhofer & Steigemann, 1975), although they are influenced by the refinement program or the scheme of constraint or restraint. In tosyl-α-chymotrypsin and elastase the angles in Pro are usually larger than the mean value, while those of the β-branched residues, Val, Ile and Thr, are smaller than the mean value. On the other hand, the oligopeptide crystal structures have shown that $\tau(C^\alpha)$ angles depend significantly on the main-chain conformations as well as the side-chain structures (Ashida, Tanaka & Yamane, 1981). For instance, $\tau(C^\alpha)$ of the second residues in the type I β turn is significantly larger than 111°, but that of the type II is not, and in the β sheets the angles are usually smaller than 111° or the regular tetrahedral angle 109·5°.

The present study has made clear some significant features of $\tau(C^\alpha)$ which need to be taken into consideration for the protein structure studies. A histogram of $\tau(C^\alpha)$ for the oligopeptides is shown in Fig. 4. The mean value with its e.s.d. and the minimum and maximum values for all the residues are:

$$110{\cdot}9\,(28)° \qquad 102{\cdot}9\text{–}117{\cdot}2°.$$

This mean value itself is essentially the same as that given by Marsh & Donohue (1967). The distribution around the mean value is, however, not normal, but fairly wide and bimodal for both the nonPro and Pro residues. Even the angles in Pro, the geometry of which is constrained by the pyrrolidine ring, deviate from the mean value in a wide range, 105·9–116·7°.

The plot in Fig. 3 shows clearly that the magnitude of $\tau(C^\alpha)$ depends on ψ. Most of the values of $\tau(C^\alpha)$ for the residues with ψ close to 0° are larger than 113°; while the angles in the extended-chain region are smaller, many are even smaller than 108°. The Gly with $\varphi > 0°$ also has the same tendency if its mirror image with $\varphi < 0°$ is adopted; Pro also has the same tendency.

A simple analysis of $\tau(C^\alpha)$ against ψ and the side-chain shape shows in Figs. 5 and 6 that it is reasonable to divide the whole ψ range into three regions, I ($\psi = -50$–$30°$), II ($\psi = 30$–$100°$) and III ($\psi = 100$–$210°$). It is also convenient to divide the amino-acid residues into four groups by their side-chain shapes: Gly; Pro; Val, Ile, Thr combined; and 'others'. The ψ dependence of $\tau(C^\alpha)$ in the four groups are different. The mean angles of each group in each region are listed in Table 1. In each region $\tau(C^\alpha)$ of Gly is the largest and that of Val, Ile, Thr is the smallest; the difference between the two is about 3°.

It is remarkable that Gly, which has the least steric effect on the main-chain structure, has the largest $\tau(C^\alpha)$ when ψ is in region I, and that Pro, which in turn has the most steric effect, also shows very significant widening from the tetrahedral angle. The amino-acid residues with the side-chains branched at C^β, Val, Ile and Thr, have significantly smaller angles than those of the other groups, but they still show a clear bimodal distribution against ψ. The mean $\tau(C^\alpha)$ angle in the folded-chain region I is about 4° larger

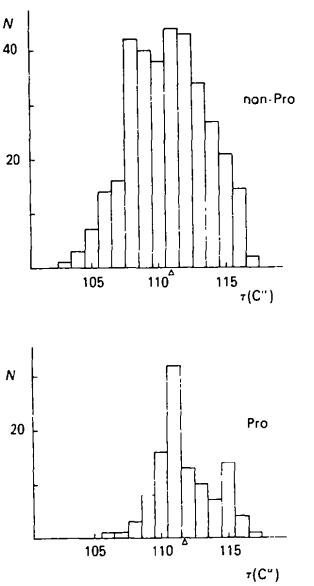

Fig. 4. $\tau(C^\alpha)$ of non-Pro and Pro.

Table 1. *Mean $\tau(C^\alpha)$ angles in three regions of ψ*

Region I: $\psi = -50$–$30°$; region II: $\psi = 30$–$100°$; region III: $\psi = 100$–$210°$ ($-150°$).

	Region	$\langle\tau(C^\alpha)\rangle$(°)	σ(°)	Max (°)	Min (°)	Number
Gly	I	115·1	1·5	117·2	110·8	27
Gly	III	110·7	2·0	115·3	105·8	67
Pro	I	114·3	1·3	116·7	110·8	33
Pro	III	110·7	1·4	115·0	105·9	82
Others	I	113·0	1·3	116·2	108·5	72
Others	III	109·0	2·0	113·9	104·2	89
Val, Ile, Thr	I	112·2	1·1	114·4	110·4	10
Val, Ile, Thr	III	108·0	1·2	110·5	104·9	39
All	I	113·6	1·4	117·2	108·5	142
All	II	108·3	2·4	111·2	102·9	27
All	III	109·8	2·0	115·3	104·2	277

Only the residues with $\varphi < 0°$ are included except for Gly, for which the angles of the enantiomorphs of the residues with $\varphi > 0°$ are also included. Others includes all residues other than Gly, Pro, Val, Ile and Thr. The residues in region II are so few that only the mean value for 'all' is given.

than that in the extended-chain region III for every group.

In conclusion, the $\tau(C^\alpha)$ angles depend on ψ as well as on the side-chain shapes. In the folded peptide chains in region I the $\tau(C^\alpha)$ angles need to be widened to release close contacts between the main-chain atoms of the neighboring residues. On the other hand, in the extended chains, the contacts between the neighboring residues are not so close. Thus, the $\tau(C^\alpha)$ angles need not be large, but the contacts between the neighboring side chains sometimes make the angles even smaller than the regular tetrahedral angle. This fact should be taken into consideration in protein structure refinement or theoretical model building of proteins.

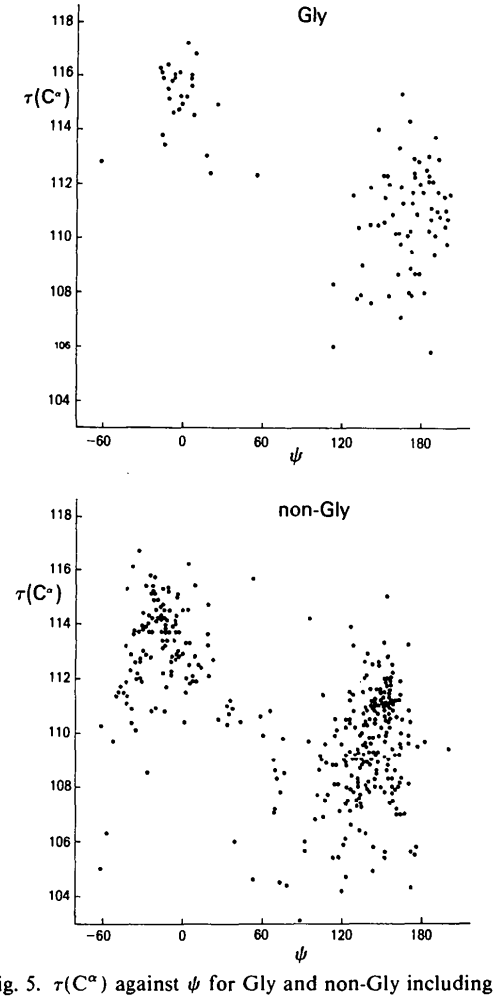

Fig. 5. $\tau(C^\alpha)$ against ψ for Gly and non-Gly including Pro.

Side-chain conformation

The conformations of the C^α–C^β bonds were studied using all the 356 data available including those of the small cyclic peptides and the (one or both sides) unblocked amino-acid residues. The three ideal staggered conformations of the bonds in peptides have a

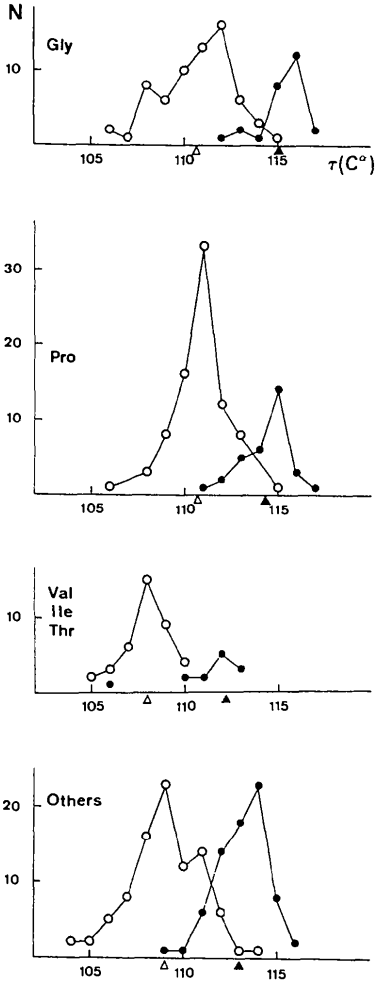

Fig. 6. Distributions of $\tau(C^\alpha)$ against ψ regions I and III for Gly, Pro, (Val, Ile, Thr combined) and others: filled circles for region I and open circles for III; triangles show the mean angles.

χ^1 of any one of ±60 and 180°:

g^-: $\chi^1 \sim -60°$, C′–C^α–C^β–C^γ *trans*,

t: $\chi^1 \sim 180°$, N^α–C^α–C^β–C^γ *trans*,

g^+: $\chi^1 \sim 60°$, H^α–C^α–C^β–C^γ *trans*.

It is found that χ^1 (and $\chi^{1,1}$) distributions have more or less similar characteristics for various amino-acid side chains except Pro, and a combined distribution curve for χ^1 (and $\chi^{1,1}$) for all the residues is shown in Fig. 7. It is clearly shown that the conformations of the C^α–C^β bonds are fully constrained to the three staggered ones. For all the data, the maximum deviation of χ^1 (and $\chi^{1,1}$ and $\chi^{1,2}$) from the ideal angles is only 27°; 73 residues have deviations larger than 10°, and only 6 deviate more than 20°. Therefore, even a single side chain in an eclipsed form with χ^1 or $\chi^{1,1}$ close to 0, 120 or 240° could not be found. Of the three staggered conformations g^- occurs most frequently and g^+ least frequently; the ratio $(g^+ : t : g^-)$ is roughly (1:2:3).

An analysis of the C^α–C^β bond conformations in globular proteins was made by Bhat, Sasisekharan & Vijayan (1979) on the basis of 23 proteins available

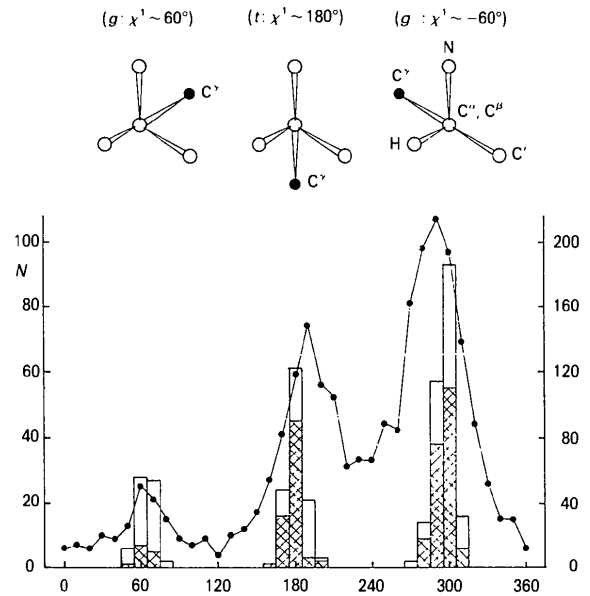

Fig. 7. The combined distribution of χ^1, in histogram with the left-hand scale, for all the amino-acid residues in oligopeptides and amino acids except for Pro, where only $\chi^{1,1}$'s are included for Val, Ile and Thr: the shaded areas represent those of the residues having both amino and carboxyl sides blocked, the open areas the (one or both sides) unblocked residues. Filled circles with the right-hand scale show the χ^1 distribution in proteins given by Bhat, Sasisekharan & Vijayan (1979). Three ideal staggered conformations viewed down the C^α–C^β bond are also shown.

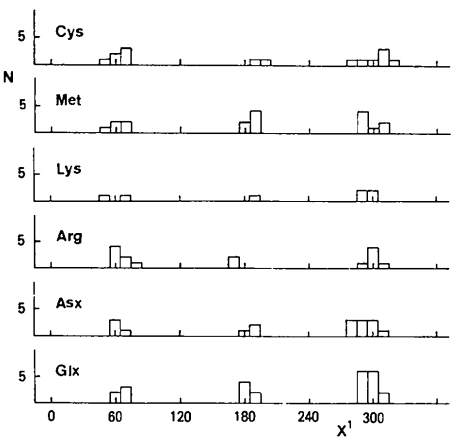

Fig. 9. Distribution of χ^1 for the long side chains.

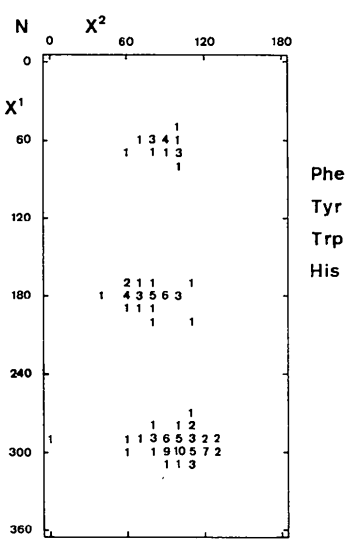

Fig. 8. Joint distribution of χ^1 and χ^2 for Phe, Tyr, Trp and His.

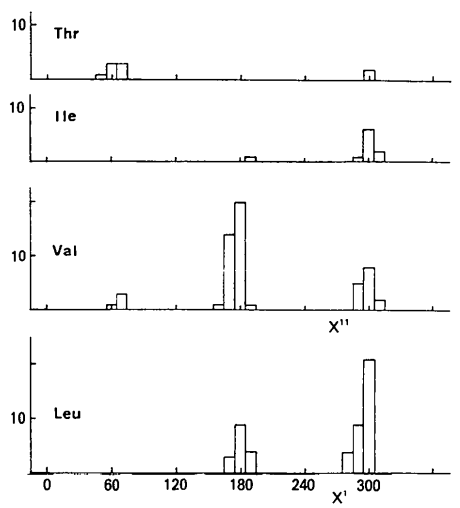

Fig. 10. Distribution of χ^1 and $\chi^{1,1}$ for the branched side chains.

in 1976. Their combined distribution curve is reproduced with filled circles in Fig. 7. Their relative peak heights for the ideal staggered conformations are quite similar to the present one of the oligopeptides. In proteins, however, the eclipsed conformation with χ^1 close to 240° occurs very frequently, even more frequently than the staggered one with χ^1 close to 60°. The probability of finding other eclipsed forms with χ^1 close to 0 or 120° is also not negligible. This fact will suggest that schemes of constraint or restraint that are too weak are (or had been) generally in use in the refinements of the side chains of poor electron density. Stronger constraint or restraint schemes for the staggered conformations should be adopted for analyses at low resolution, and for residues that have poor side-chain electron densities.

Several other characteristics of the side-chain conformations found in this study are:

(1) Phe, Tyr, Trp, His: for χ^1 the ratio of occurrences of $(g^-:t:g^+)$ is (4:2:1); and χ^2 is $90\pm30°$ (Fig. 8).

(2) Glx, Asx, Arg, Lys, Met, Cys (all having long side chains): for χ^1, g^+ occurs rather more frequently than t (Fig. 9).

(3) Glx, Arg, Lys: χ^2 is mostly t.

(4) Glx: $\chi^3 = -30$–$50°$, in many cases the side chain including the carboxyl group is nearly planar; Asx: $\chi^2 = -90$–$90°$.

(5) Leu: $(\chi^1, \chi^{2,1})$ is mostly (g^-, t) or (t, g^+), the ratio between the two is (2:1) (Fig. 10).

(6) Val: $(g^-:t) = (1:2)$ for $\chi^{1,1}$ (Fig. 10).

(7) Cys: χ^3 (C^β–S–S–C^β) is found in the two regions 81 ± 15 and $-82\pm2°$.

(8) Thr, Val, Ile and Leu: the mean difference between $\chi^{n,1}$ and $\chi^{n,2}$, where n is 1 or 2, is 123°.

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