Structure of beta sheet

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A beta-pleated sheet is an example of a protein tertiary structure. Chemical structure of beta-sheet. Protein structure of beta sheet. The alpha-helix and beta sheet are examples of protein structure. Crystal structure of beta-sheet. Beta pleated sheet structure of protein. Structure of beta pleated sheet. The beta pleated sheet structure of protein is due to.

Introduction to Protein Structure Secondary Structure -- Beta Sheet The backbone of a beta sheet (shown in colour below) is arranged in the zig-zag (or folded mode). Notice how the side chains (shown in dark grey) attach to the spine on each side of the sheet.The following example is a three-wire beta sheet. At least two strands are needed to define a beta sheet; many beta sheets have more strands. The beta sheet is stabilized by hydrogen bonds between the carbonyl oxygen of an amino acid in one filament and the nitrogen of the spine of a second amino acid in another filament. Beta sheets may be parallel or antiparallel. If the amine terminal residue of each filament “pointed” in the same direction, the sheet is considered parallel. Antiparallel sheets have amine terms that “point” in opposite directions. Is Turn on the “highlight” in the figure below to color the amine terminal residue of each filament. On Off H-bonds highlight the side chains This beta sheet consists of residues 42-46, 49-54 and 56-60 in chicken egg white lysozyme. Copyright Ã˜Â¿Â½ 1998, 1999, 2007 by Frank R. Gorga;Ã Page maintained by F.R. Gorga;Ã Last updated: 12-Mar-2007 Illustrated glossary of organic chemistry representations of a protein Ã˜Â¿Â½-sheet Ã Ã˜Â¿Â½ For individual amino acids, a PÃ˜Â± of 1.1 denotes a Î±-helix favored amino acid, and values between 0.9 and 1.1 indicate that the amino acid is neutral in this respect [31]. The same principle applies to P12. The amino acid propensities calculated using our data set (PÃÂ± i and PÃ2 i) are shown in Table 2. Their standard deviations ranged from 0.001 to 0.004. The results agree with previous reports [1, 6, 10]. Table 2 Average amino acid propensities for the Ã©Â±elic and Ã©2-strick conformation We have also calculated the amino acid propensities for the exposed and buried residues (Pexp i and Pbur i) in the secondary structural elements (Table 2). For the propellers, the three average propensities PÃ©Â± i , PÃ©Â±exp i and PÃ©Â±bur i have similar tendencies. On the other hand, the mean propensities for exposed residues (P12exp i) and for buried residues (P12bur i) for yarn 2 differ significantly (Table 2). It is particularly interesting to note that Lys and Arg, but not two other charged residues, Asp and Glu, are preferable as residues exposed in Î2 filaments. Not surprisingly, all charged amino acids are disadvantaged as residues buried in filaments Ã©2. Buried regions do not favor the charged amino acids for the Ã©2 yarns, while the Ã©Â±-helix can tolerate the charged amino acids.As previously reported in statistical studies, charged amino acids (including Lys and Arg) give low values of PÃ©2[1, 6, 10, 13], which is in agreement with the mean propensities, PÃ©2 i , determined in this work. Ours However, they show that Lys and Arg have relatively high PI2exp values for exposed residues, but this property is masked when comparing average propensities. In our data set, the fraction of residues exposed in the Ã©2 yarns is low low low Î±-helices (46%). Most of the residues in Î2-strands are buried within proteins and covered by Î±-helices or loop regions; the exposed residues are therefore less frequently encountered in Î2-strands, and their contributions to the mean PÎ2 are therefore small. Jiang and colleagues [10] have suggested that hydrophobicities of amino acid side chains are the key determinant of Î2 sheet structures, but our data suggest that this is true for buried residues but not for residues exposed in Î2 sheet structures. Minor and Kim [27] measured the propensity of the 20 amino acids for Î2-foil formation in a variant of the IgG-binding domain of protein G, which have four antiparallel Î2-strands. The amino acid substitutions were performed at a host site on the solvent-exposed surface of the central wire. The propensities of those experiments show a strong correlation with the logarithmic PÎ2expi values obtained here (R = 0.82), although they show a weaker correlation with our logarithmic PÎ2bur values (R = 0.63). Moreover, there is a poor correlation between the propensities determined by Minor and Kim [27] and those of Chou and Fasman [1]. These results show that the preference for Î2-strands differs for exposed and buried sites. Foldable dependence of amino acid propensities for Î±-helices The amino acid propensities in the helical region of fold j, PÎ± ij , and the region Î2-strand of fold j, PÎ2 ij , have been calculated for 39 and 24 SCOP folds, respectively (Figure 1). Their standard deviations range from 0.01 to 0.05. With the exception of Met, Cys, Trp, Asn, Asp and His for PÎ± ij , and with the exception of Met, Pro and Cys for PÎ2 ij , the amino acid population differed (confidence level >90%) by more than a couple of folds. Figure 1Amino acids propensities for each fold SCOP. Amino acid plots for each SCOP fold for Î±-helices (A) and Î2-strands (B). Each box contains 50% of the data with the median value displayed as a line. The upper and lower part of the box mark the limits of Â±25% of the data. The lines extending from the top and bottom of each cell mark the minimum and maximum values within the data set that fall within an acceptable range. Any value outside this range, called an outlier, is displayed as an individual point. The underlining of some residues (one-letter code) on the horizontal axis indicates that the results of the Fisher-Irwin population proportion test indicated that the differences in propensity are statistically significant between folds. In particular, a wide range of PÎ± ij values was obtained for the aromatic residues Phe (0.66â2.00) and Tyr (0.58â1.89), depending on the type of fold, and the average bending propensity for all folds is about 1.0 for these amino acids (Figure 1A and Table 2). The propensities of the loaded residues Lys and Arg (0.80–1.71) varied widely depending on a fold. On the other hand, in >80% of the SCOP, Leu or Glu folds are favored inconformation, while Val, Pro, Ser, Thr, Asn, Asp and Gly are uncomfortable. Wing is favored in the Î±-helix conformation in most folds (79%) but is disadvantaged in two folds (protein kinase-like and 4-helix cytokines). In particular, the value of the propensity of wing for the fold “4-helix cytokines” is quite low (PÎ± ij = 0.64). Met, Cys, Trp, and His do not have a fold population difference at the >90% confidence level in any pair of folds, although their propensities vary widely between folds. Therefore, we have not further evaluated these amino acids. Richardson et al. showed that Ala is not favored in Î±-helix ends [7], suggesting that a short Î±-helix does not favor Ala. The average Î±-helix length of the fold of 4 helical cytokines is, however, the third longest of those of 39 folds (the longest and the second longest are those of “Ferritin-like” and “Four-helical up-and-down bundle”, respectively). Then, the correlation coefficient between the average length of Î±-helix and amino acid propensity for each amino acid were calculated, so that they were smaller than 0.4. This result indicates that there is no relationship between the average Î±-helix length and the helical propensity of any amino acid. Engel et al. shows that most helices are amphiphilic [7, 12], suggesting that the propensities for Î±-helix depend on the fraction of exposed residues. Thus, we examined correlations between the fraction of exposed residues and the frequency of amino acids in Î±-helices. No amino acid showed a strong correlation (R < â0.7 or R > 0.7) between the fraction of exposed residues and amino acid frequency, although the loaded residues, Lys and Asp have a relatively strong positive correlation (RK = 0.66, RD = 0.54). In contrast, the correlation coefficients of Glu and Arg (also loaded amino acids) are small (RE = 0.26, RR = 0.07). Figure 2 also shows propensities for exposed and buried amino acids for each SCOP fold. For exposed regions of an Î±-helix (Figure 2A), fewer than ten amino acids show the difference in population with 90% confidence for at least a couple of folds. This is probably due to the fact that the dataset was limited to exposed residues. Gl (PÎ±exp ij: 1.0Å-1.92) is favoured in exposed areas (Figure 2A) while Leu (PÎ±bur ij: 0.97Å-1.88) is favoured in buried areas (Figure 2B) for more than 80% of folds. Pro and Gly are extremely unfavourable in both exposed and buried regions for more than 92% of the folds. Ala propensities in exposed and buried regions of Î±-helix have a similar tendency to PÎ± ij . Ala is favoured in the Î±-helix conformation in exposed and buried regions for 72% and 79% of folds, respectively, while Ala is disadvantaged for 8% and 13% of folds, respectively, when exposed or buried. For the fold “cytokines 4-helix”, also the of the wing propensity in the exposed and buried regions are low (Pαexp ij ije PÃ±bur ij Ã”Â¡=Â¡Â¡Â¡Â¡Â¡0.60). For the aromatic residues Phe and Tyr a wide range of PÃ©Â±bur ij values were obtained, depending on the type of fold (Figure 2B), as well as PÃ©Â± ij values.Figure 2Amino acid sensitivities to exposed and buried residues. Charts of amino acid propensities for each SCOP fold for exposed (A) and buried (B) residues in the Æ±elics and for exposed (C) and buried (D) residues in the Æ2 filaments. Propensities for Ã2 yarns for Trp in the SCOP Â "PHÂ" fold and for Lys in the SCOP Â "protein kinaseÂ" fold were out of range (4.3 in C and 3.8 in D, respectively) and are not shown. The underlining of some residuals on the horizontal axis denotes that the results of the Fisher-Irwin population proportion test indicated that differences in propensities are statistically significant between folds. As shown in Figure 1B, a wide range of PÂÂ² values ij was obtained for Trp (0.45Ã¢2.22), Thr (0.73Ã¢1.87), Lys (0.46Ã¢1.45) and Arg (0.51Ã¢1.42) depending on the fold type. For Lys, although PÃ¢² ij was Ã¢1.2, which had population differences corresponding to the 90% confidence level with that of other folds. These three folds are all ÃÂ²Â¢â'¬â"¢ or Â¢â'¬â"¢+Â¢â'¬â"¢, and all have largely exposed ÃÂ²Â¢â'¬â"¢ filaments, whereas ÃÂ²Â¢â'¬â"¢ filaments are usually covered by ÃÂ±-helical or loop regions, especially in Ã¢â'¬â"¢/ÃÂ²Ã¢â'¬â"¢ proteins (Table 1). It has long been thought that Â²-files prefer hydrophobic residues [1, 6, 10]; however, it now appears that widely exposed Â²-sheet structures prefer hydrophilic residues such as Lys. In contrast, the four amino acids Val, Ile, Phe, and Tyr are favored (PÂÂ² ij Ã¢>Ã¢1.1) in ÃÂ²-fold over 80% of folds, with Val (1.40Ã¢2.68) and Ile (1.17Ã¢2.33) having particularly high propensities in this regard. The six amino acids Pro, Ala, Asn, Asp, Glu, and Gly are disfavored (PÃÂ² ij Ã¢â1.1) for more than 75% of the folds, indicating that these amino acids, which have a branched or aromatic lateral chain, are favored in the exposed regions of Î2-strands in all types of folds. On the contrary, the amino acids that are unfavored in all the folds in Î2-strands are Pro (0.22â0.87), Ala (0.28â0.70) and Gly (0.23â0.88) for the exposed regions, and Pro (0.12â0.87) for the buried regions. It is interesting that PÎ2exp ij values for all folds for Ala are lower by comparison (PÎ2exp ij ¤

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