Common substructures and sequence characteristics of sandwich-like proteins from 42 different folds.

Kister A.E. Department of Mathematics, Rutgers University, Piscataway, NJ, USA.

Abstract

This study addresses the following fundamental question: Do sequences of protein domains with sandwich architecture have common sequence characteristics even though they belong to different superfamilies and folds? The analysis was carried out in two stages: determination of substructures in the domains that are common to all sandwich proteins; and detection of common sequence characteristics within the substructures. Analysis of supersecondary structures in domains of proteins revealed two types of four-strand substructures that are common to sandwich proteins. At least one of these common substructures was found in proteins of 42 sandwich-like folds (as per structural classification in the CATH database). Comparison of the sequence fragments corresponding to strands that make up the common substructures revealed specific rules of distribution of hydrophobic residues within these strands. These rules can be conceptualized as grammatical rules of beta protein linguistics. Understanding of the structural and sequence commonalities of sandwich proteins may also be useful for rational protein design.

Keywords: Secondary structure, Supersecondary structure, Sandwich substructures, Sandwich architecture, Sequence comparison, Structural bioinformatics, Contacts between beta-strands, Beta protein linguistics.

Introduction

According to the protein structural hierarchical classification adopted in the CATH database, ‘architecture level’ is a general description of the gross arrangement of secondary structures that is independent of their connectivity.¹ Thus, a particular architecture may describe structures from non-homologous superfamilies with different numbers of secondary structure elements and diverse connectivity. Examples of protein architecture are beta-sandwich or beta-barrel. An important unanswered question is whether any specific sequence features are responsible for the specific protein architecture. This study focuses on the relationship between sequences and protein structures with sandwich-like architecture. Sandwich folds in beta-protein domains are characterized by two main beta sheets packed against each other. This architecture characterizes more than 40 protein folds and 532 superfamilies in the CATH database structural classification of protein domains. Immunoglobulin-like and Jelly Rolls folds have the largest number of superfamilies: 318 and 127, respectively.

Usual methods for detecting sequence similarity using similarity scores²⁻⁴ have not so far been successful in uncovering common sequence characteristics in the highly non-homologous sandwich proteins. In this study, an alternative, two-stage approach to uncovering sequence similarities is proposed. The first stage is to identify ‘substructures’ common to proteins of all sandwich folds. Substructures are defined as specific arrangements of two pairs of consecutive strands in two main beta-sheets. The four-strand substructure represents the smallest possible sandwich structure. One example of such a substructure – ‘the interlock’ - was previously shown to be present across a group of sandwich-beta proteins from different superfamilies and protein folds.⁵ Here we describe

another type of conserved arrangement of four strands within sandwich-like folds proteins. We show that at least one of these two types of substructure is always present in sandwich-like proteins. Since these substructures are an invariant feature of sandwich proteins, their formation is likely a necessary condition for the development of structures with this architecture.

The second stage of analysis is to find common sequence characteristics within the strands that make up the conserved substructures (the ‘substructure strands’). Numerous lines of evidence point to the decisive role of hydrophobic residues in beta-sheet formation of beta structures. Hydrophobic residues (a) have a special propensity for beta sheets;⁶⁻⁸ b) play a key role in the formation of ‘hydrophobic zipper hypothesis’;⁹ c) are mostly responsible for protein folding and stability;¹⁰⁻¹¹ and d) the development of hydrophobic core;¹²⁻¹⁴; and, e), are also important for the formation of β -sheet packing interfaces.¹⁵ Therefore, the analysis of substructure strands focuses on the locations and contacts of hydrophobic residues in sequences. Because contacts between oppositely charged residues – ‘salt bridges’ - also significantly contribute to protein stability,¹⁶⁻¹⁷ these interactions were also taken into account in our analysis.

As the standard alignment procedures did not reveal conserved hydrophobic positions in sequences from different superfamilies, our analysis focused on the finding of pairs of hydrophobic residues that form contacts between substructure strands. We identified such contacts that are invariably present in substructures of sandwich-like proteins. The matrix of conserved contacts can be regarded as the common sequence characteristic of sandwich proteins. Another characteristic feature of the substructures is the relatively large proportion of hydrophobic residues in the substructure strands.

Analysis and Results

Two types of conserved supersecondary substructures in sandwich domains

Substructure type 1 is formed by four consecutive strands. Two strands ($i-1$ and i) form backbone hydrogen bond contacts in one sheet and the other two strands ($i+1$ and $i+2$) form hydrogen bond contacts in the other sheet (Fig. 1). Two variants of this substructure, subtype 1a, and 1b, differ in the relative locations of strands $i-1$ and $i+2$ as shown in Fig. 1a and 1b, respectively. Substructure 1a was found in 20 folds and substructure 1b - in 10 folds (Table 1, columns “SubS 1-4”).

Substructure Type 2 has two pairs of consecutive strands: i and $i+1$, and j and $j+1$ (Fig. 2). Two consecutive strands in each pair are located in different beta-sheets, e.g. strand i is located in one sheet and strand $i+1$ is in the other sheet. The strands from the different pairs are neighbors in the same sheet and share backbone hydrogen bond contacts, e.g. strand i and j are located next to each other in sheet A and strands $i+1$ and $j+1$ - in sheet B. The four possible variants of substructures type 2 – subtypes 2a, 2b, 2c, and 2d - are shown in Fig 2a-d, respectively. Substructure 2a is found in 23 folds, 2b – in 3 folds, 2c – in 8, folds, 2d - in 32 folds (Table 1, column “SubS 1-4”).

Substructures in sandwich folds. At least one type 1 or type 2 substructure was found in each domain (Table 1). Most domains contained 2-4 substructures. These restrictions found in the arrangement of substructure strands significantly reduce the number of possible variants of SSS in sandwich domains.

There are two specific characteristics of the substructures. First, the four strands in the substructures form the smallest possible sandwich protein domain. Secondly, SSS

substructures describe almost all the observed arrangements of consecutive strands are located in different beta-sheets. There were a total of 166 such pairs of consecutive strands in the examined structures, of which 151 pairs were described by the substructures. For example, in structure 1h8e (Table 1, CATH fold 2.60.15, column 'SSS domain'), the arrangements of consecutive strands 2 and 3, 5 and 6, 7 and 8, and 9 and 10 are described by substructures 1b, 2c, 1a, 2c, respectively (Table 1, columns 'SubS 1-4'). One exception in this structure was found for consecutive strands 4 and 5 in two different beta-sheets that are not part of a conserved substructure. Sequential strands that are located in different sheets but are not substructure strands were found mainly at the edges of the beta-sheets.

Sequence analysis

Pairs of contact residues (PCR). To uncover common sequence characteristics in widely dissimilar proteins from different folds, the concept of 'Pairs of Contact Residues' (PCR) was introduced. PCR is defined as the pair of residues that are located opposite each other on two neighboring strands within one beta-sheet. For the pair of antiparallel strands $i-2$ and $i-1$ shown in Fig. 1a, examples of PCRs are pairs of residues 1 and 5, 2 and 4, etc). If there is a 'bulge' in a strand, then residues that make up the bulge are not eligible for PCRs. For example, in table 2a (structure 1h8e, fold 2.60.15) residue F28, which make up the bulge in strand #2 (sheet A) has no opposite residue in strand # 1. Thus, the total number of PCRs in pair of strands #1 and 2 is seven, as shown in Table 2a, the column "Characteristics pair of strands", in square parenthesis.

Hydrophobic residues in substructures. The total number of hydrophobic residues was equal to, or greater, than the total number of PCRs in about 75% of the substructures. In

18% of substructures, the total number of hydrophobic residues is one less than the total number of PCRs (Table 1, columns “SubS 1-4”). These observations highlight the high proportion of hydrophobic residues in the substructure strands.

A subset of PCRs in which both residues are hydrophobic was called ‘Pairs of Hydrophobic Residues’ (PHRs). The total numbers of PHRs in all substructures of the sandwich domains varied from about 25% to 50% of the total number of PCRs. In 88% of the substructures, the number of PHRs varied from 3 to 7 (Table 1, columns “SubS 1-4”).

Additional evidence for the importance of specific distribution hydrophobic residues to structure formation derives from the location of residues in strands of beta sheets A and B (see columns sequences of strands in Table 2a and 2b). Residues forming PHR are located directly one below each other, which corresponds to the actual location of the strands relative to each other in the beta-sheet. The representations of residues showed that a significant number of hydrophobic residues are not randomly distributed in beta sheets, but most are in columns with predominantly hydrophobic residues in all substructures (see framed PHRs in the columns ‘sequences of strands in beta-sheets A and B’ in Table 2a and 2b).

Pairs of charged residues. Protein folding initiation sites contain not only hydrophobic amino acids but also charged residues.¹⁸ Thus, pairs of oppositely charged residues were taken into account in order to uncover the common sequence elements of sandwich-like proteins. The pairs of charged residues were found in almost 20% of neighboring substructure strands in the same sheet. (Table 2a, b in the columns “Sequences of strands in beta-sheets A and B”).

Inter-sheet contacts of hydrophobic residues within substructures. A Pair of Hydrophobic Residues that form inter-sheets contacts was called PHR-IC. The numbers of PHR-ICs for each substructure are shown in square brackets in the column “Intersheet Contacts” (Tables 3 and 4). At least one PHR-IC was found in all substructures, and most substructures have 3 and more PHR-ICs. The residues of PHR-IC are shown in columns “Residue-residue intersheet contacts (PHR-IC)” in Table # 3 and 4. Hydrophobic residues that comprise PHR determine mutual orientation between pairs of strands in beta sheets, while residues that make up PHR-IC define the relative orientation of beta-sheets. It was found that a residue of at least one PHR is involved in intersheet contact. Thus, the dependence of the formation of PHR in 2D sheet and PHR-IC in 3D sandwich structure on the distribution of hydrophobic residues in amino acid sequences can serve as one of the decisive criteria for the relationship between primary, secondary, and tertiary structures.

Discussion

Prerequisites for the formation of sandwich structures. All analyzed structures with the sandwich architecture contained at least one conserved substructure of the type shown in Fig. 1 and 2. Thus, the two types of substructures, with their specified arrangements of four strands, may be considered as a prerequisite for the formation of two sheets in sandwich-like protein domains. It is plausible to suggest that the strands are reorganized in space to form the substructure(s) as the critical early step in the formation of hydrophobic core between sheets. The sandwich substructures can be considered as the structural nucleus of protein domains, while non-substructure strands are the ‘annexes’ of protein substructure(s). The presence of the structural nucleus provides indirect evidence that proteins of various topologies in sandwich architecture are either evolutionarily related or are the result of

convergent evolution, in which two types of substructure independently formed as indispensable structural elements of stable sandwich domains.

Similar sequence characteristics of substructures.

Identification of the common supersecondary structure characteristics of sandwich proteins - the substructures - allowed for the determination of the common sequence characteristics of sandwich proteins. These common sequence characteristics are the specific distribution of hydrophobic residues in sequences of proteins with sandwich architecture. The essential role of hydrophobic residue interactions in determining the pathway of protein folding is supported by many studies.^{12, 19}

The distribution of hydrophobic residues in the substructure strands in the same beta-sheet can be characterized with respect to:

a) The proportion of hydrophobic residues with a tendency to form beta strands ('preferred' residues). The ratios of preferred and non-preferred residues for strands, adjusted for strand length of the strands were considered in our recent work²⁰;

b) A tendency to form PHR and pairs of oppositely charged residues. Ability for form pairs of hydrophobic or charged residue contacts depends on relative positions of respective residues in the neighboring strands in a beta sheet. This imposes great restrictions on the distribution of these residues in the sequence.

c) The proportion of hydrophobic residues located in 'inward-oriented' positions in beta-strands. Most residues involved in PHR were found in these inward-oriented positions and formed PHR-IC.

It can be argued that the similarity of sequences in sandwich substructures is determined not only by the number of conserved positions with similar residues as a result of artificial alignment procedures, but rather by the distributions of hydrophobic residues in the substructure strands in conformance with the above requirements. The algorithm for the distribution of residues in substructure sequences also impose certain limitations on the arrangement of hydrophobic residues in the non-substructure strands (see framed PHRs in the columns ‘sequences of strands in beta-sheets A and B’ in Table 2a, b).

The specific rules of distribution of hydrophobic residues within the substructures are characteristics of sandwich proteins but are not a sufficient criterion to classify structure as having sandwich architecture. The sequence template for a particular sandwich topology includes not only the rules of distribution of hydrophobic residues within the substructure strands but also the specifications of the minimum required the number of residues with high-frequency adjusted for the lengths of strands and loops respectively. These data can be obtained from statistical analysis of residues of strands and loops in all beta proteins. It was shown that these sequence characteristics are very specific and sensitive for identifying proteins of a given fold from all known protein sequences.²⁰

Beta-Protein linguistics in substructures. The term ‘protein linguistics’ is often used due to the numerous parallels between linguistics and biology.²¹⁻²⁹ Human linguistics analyzes how letters of the alphabet form meaningful texts, while protein linguistics analyzes how a sequence made up of 20 amino acids ‘letters’ forms a stable and biologically active three-dimensional structure. In linguistics, as in biology, the essential problem is to identify laws that determine the nonrandom arrangement of elements in sequences. Linguistics usually considers a three-level scheme of analysis: Letter → Word → Sentence. These levels of

analysis can be applied to biological languages as well. The letters are conditional symbols that designate sounds in written human languages or the monomers of polypeptide chains in protein languages.

The problem of defining ‘word’ and ‘sentence’ is more complex. One of the best-known definitions for a word in linguistics was introduced by Bloomfield: the word is the "smallest free form", i.e. a form that can occur alone as an expression.³⁶ In the protein linguistics, the definitions of ‘word’ and ‘sentence’ differ depending on the objectives of the study. For example, to analyze the location of domains in a multi-domain structure, domains can be considered ‘words’, and the tertiary structure of a protein - ‘sentence’.³⁷⁻³⁸ If the goal is to analyze the sandwich-like domain then the protein domain can be regarded as a ‘sentence’.

For our purposes, in beta-proteins linguistics two adjacent strands in a beta-sheet may be considered a ‘word’ because they make up the smallest part of the beta-sheet that can exist independently. Thus, in beta-protein morphology, the ‘word’ consists of two sequence fragments that are separated by a string of residues. (Note, in alpha protein linguistics a single helix can be considered as a ‘word’.)

Our study focused on a four-strand “mini-sandwich” substructure that can exist as an autonomous domain or as part of a domain with more than four strands. Such a substructure can be regarded as an independent ‘clause’ in beta-protein linguistics since independent ‘clause’ in human linguistics is a part of the sentence that can stand alone as a sentence.

The next level of language complexity is syntax — rules that govern the arrangement of words to create grammatically correct clauses and sentences. Protein syntax determines the formation of a substructure and, ultimately, a stable and functionally viable three-dimensional

structure. If a word consists, for example, of two strands i and j (Fig. 2a) then a 'half-word' - strand i - may be a neighbor of the other strand m which participates in the formation of another word: $m - i$. Thus, one strand could be a part of two words, e.g. strand j can be part of $i - j$ word as well as $j - k$ word. Therefore, the beta-sheet is a set of words that are partially enclosed in each other. This design fortifies the structure of the beta-sheet.

We can deduce some of the rules that govern the process of converting a 1D sequence of residues into 'words' and then into a 'meaningful' 3D sandwich structure that is stable and capable of performing biological functions. These rules can be formulated as follows:

1. For each beta-protein word (a pair of H-bonded strands in a beta-sheet) one can estimate the minimum allowed the number of letters (residues) favorable for word formation and the maximum allowed the number of letters that are unfavorable to word formation. These conditions are determined based on the statistical analyses of residues in strands in all beta proteins.

2. Whether a sequence fragment can form a word will depend on the coordinated arrangement of hydrophobic residues in a fragment, which will determine the possibility of PHR formation in a word. The coordinated arrangement of pairs of oppositely charged residues is also frequently observed in words.

3. Syntax rules determine the relative position of words in two beta sheets to ensure the stability of the substructure. The condition is the location of most hydrophobic residues in both words at positions in which the residues can form intersheet contacts. In all examined substructures there is at least one PHR in which both residues are directed inward.

Material and Methods

Structural analysis. The sandwich architecture in the CATH database encompasses 44 protein folds¹. Proteins of two folds (2.60.460 and 2.60.530) were not included because structural classification in PDBSum database³⁰ does not support sandwich-like architecture for proteins in these two folds. Thus, 42 folds, which describe 528 protein superfamilies, about 40% of all beta-protein superfamilies, were interrogated. One protein domain from every fold, which served as the representative for its respective fold in the CATH database, was examined. For secondary structure analysis, the information about localization of strands in sequences was taken from PDB.³¹ For supersecondary structure (SSS) of the domains, PDBsum topology diagrams that show the arrangement and connectivity of strands in beta sheets were used.

The strands in the domains were numbered starting at the N-terminus. The SSSs are presented according to their arrangements in the two beta sheets (Table 1, column ‘SSS domain’). For residue-residue contact analysis, CSU software was used, which calculates contact surface area for all atoms in residues and provides detailed description of contacts.³²

Definition of hydrophobic residues. Our analysis focuses on hydrophobic residues Ile, Val, Leu, Phe, Met, and Trp in strands. Residues Ala, Tyr, and Cys were added to the group of hydrophobic residues because they often substitute for hydrophobic residues in strands. The weakly hydrophobic Ala is considered both “interior-seeking” and “water-seeking” according to many hydrophobic scales.³³ Although Tyr has both polar and nonpolar groups, it often substitutes for hydrophobic residues in strands and is classified as a hydrophobic amino acid on most hydrophobicity scales.³⁴ Cys residue can play the role of a hydrophobic residue in specific protein microenvironments.³⁵

References

1. Orengo CA, Michie AD, Jones S, Jones DT, Swindells MB, Thornton JM. (1997) CATH- a hierarchic classification of protein domain structure Structure 5(8):1093-108.
2. Heringa, J. (2008) Sequence Similarity. In: Encyclopedia of Life Sciences (ELS).
3. Chatzou M, Magis C, Chang JM, Kemena C, Bussotti G, Erb I, Notredame C. (2016) Multiple sequence alignment modeling: methods and applications Brief Bioinform 17(6):1009-1023
4. Le Q, Sievers F, Higgins DG.(2017) Protein multiple sequence alignment benchmarking through secondary structure prediction. Bioinformatics. 33(9):1331-1337
5. Kister, A.E., Finkelstein A.V., Gelfand, I.M. (2002) Common features in structures and sequences of sandwich-like proteins. Proc Natl Acad Sci U S A. 99:14137-14141
6. Chou PY, Fasman GD., 1974, Conformational parameters for amino acids in helical, beta-sheet, and random coil regions calculated from proteins. Biochemistry 13(2), 211-222.
7. Fujiwara K, Toda H, Ikeguchi M. (2012) Dependence of α -helical and β -sheet amino acid propensities on the overall protein fold type. BMC Struct. Biol.12:18.
8. Costantini S, Colonna G, Facchiano AM. (2006) Amino acid propensities for secondary structures are influenced by the protein structural class. Biochem Biophys Res Commun. 342: 441-451
9. Dill KA, Fiebig KM, Chan HS. (1993) Cooperativity in protein-folding kinetics. Proc. Natl. Acad. Sci. U S A. 90: 1942-1946

10. Nick Pace C, Scholtz JM, Grimsley GR (2014) Forces stabilizing proteins. FEBS Lett. 588(14):2177-84
11. Sengupta D, Kundu S.(2012) Role of long- and short-range hydrophobic, hydrophilic and charged residues contact network in protein's structural organization. BMC Bioinformatics. 13: 142.
12. Baldwin RL, Rose GD. (2016) How the hydrophobic factor drives protein folding Proc. Natl. Acad. Sci. U S A. 113: 12462–12466
13. Banach M, Konieczny L, Roterman I. (2019) Secondary and Supersecondary Structure of Proteins in Light of the Structure of Hydrophobic Cores. Methods Mol Biol., 1958: 347-378.
14. Jager M, Deechongkit S, Koepf EK, Nguyen H, Gao J, Powers ET, Gruebele M, Kelly JW. (2008) Understanding the mechanism of beta-sheet folding from a chemical and biological perspective. Biopolymers. 90:751-758.
15. Joo H, Tsai J. (2014) An Amino Acid Code for β -sheet Packing Structure Proteins. 82: 2128–2140.
16. Bosshard HR, Marti DN, Jelesarov I. (2004) Protein stabilization by salt bridges: concepts, experimental approaches and clarification of some misunderstandings.
17. Kumar S, Nussinov,R. (2002) Close-range electrostatic interactions in proteins. Chembiochem. 3: 604-617
18. Dyson HJ, Wright PE, Scheraga HA. (2006) The role of hydrophobic interactions in initiation and propagation of protein folding. Proc Natl. Acad. Sci. U S A. 103(35):13057-13061

19. Bachmann A., Wildemann D., Praetorius F, Fischer G, Kiefhaber T. (2011) Mapping backbone and side-chain interactions in the transition state of a coupled protein folding and binding reaction. *Proc. Natl. Acad. Sci. U S A.* 108: 3952-3957
- 20 . Kister A.E. (2018) Sequence pattern for Supersecondary secondary structure of Sandwich-like Proteins. *Methods of Molecular Biology.* 1958, 313-327
- 21 Buchan DWA, Jones DT (2020) Learning of a functional grammar of protein domains using natural language word embedding techniques *Proteins.* 88(4): 616-624
22. Popov O, Segal DM, Trifonov EN (1996) Linguistic complexity of protein sequences as compared to texts of human languages. *Biosystems.* 38: 65-74.
23. Gimona M. (2006) Protein linguistics – a grammar for modular protein assembly? *Nat Rev Mol Cell Biol.* 7:68-73
24. Przytycka T, Srinivasan R, Rose GD (2002) Recursive domains in proteins. *Protein Sci.* 11:409-417
25. Searls DB. (2012) A primer in macromolecular linguistics. *Biopolymers* 99: 203-217
26. Kister A.E. (2015) Amino acid distribution rules predict protein fold: protein grammar for beta-strand sandwich-like structures *Biomolecules.* 5:41-59
27. Dyrka W, Pyzik M, Coste F, Talibart H (2019) Estimating probabilistic context - free grammars for proteins using contact map constraints. *Peer J.* 7:e6559
28. Bloomfield L. (1926). A set of postulates for the science of language. *Language* 2: 153–164.

29. Yu L, Tanwar DK, Penha EDS, Wolf YI, Koonin EV, Basu MK (2019) Grammar of protein domain architectures. *Proc. Natl. Acad. Sci. U S A* 116:3636-364
30. Laskowski RA, Jabłońska J, Pravda L, Vařeková RS, Thornton JM (2018). PDBsum: Structural summaries of PDB entries. *Prot. Sci.*, 27: 129-134.
31. Burley SK, Berman HM, Bhikadiya C, Bi C, Chen L, Costanzo LD., et al. (wwPDB consortium), (2019) Protein Data Bank: the single global archive for 3D macromolecular structure data. *Nucleic Acids Research*. 47: D520–D528.
32. Sobolev V, Eyal E, Gerzon S, Potapov V, Babor M, Prilusky J, Edelman M. (2005). SPACE: a suite of tools for protein structure prediction and analysis based on complementarity and environment. *Nucleic Acids Res* 33: W39-W43.
33. Nilsson, I, Johnson, AE., von Heijne, G. (2003) How hydrophobic is alanine? *J. Biol. Chem.* 278: 29389-29393.
34. Simm S, Einloft J, Mirus O, Schleiff E. (2016) 50 years of amino acid hydrophobicity scales: revisiting the capacity for peptide classification *Biol. Res.* 49:31.
35. Nagano N, Ota M, Nishikawa K. (1999) Strong hydrophobic nature of cysteine residues in proteins. *FEBS Lett.* 458: 69-71.

Conflict of interest: The author declares no conflict of interest.

Table 1

CATH folds	Sfam	PDB code	Chain fragment	SSS domain	SubS 1	SubS 2	SubS 3	SubS 4
2.60.9	1	2hnu	A: 7-87	sheet A: 4=3=2=1 sheet B: 5=6=7=8	1a 4=3 5=6 3(8)[8]	1a * 7=8 2=1 2 (7)[8]	—	—
2.60.11	1	1occ	F:1-98	sheet A: 4=5=1 sheet B: 3=2 No SubS for strands # 1 and 2 strands # 1 and 5 are parallel	1a 4=5 3=2 4(14)[13]	—	—	—
2.60.15	1	1h8e	H: 15-103	sheet A: 2=1=9=8=5 sheet B: 4=3=6=7=10 strands #1 and 9 parallel No SubS for strands # 4 and 5	1b 2=1 4=3 4 (13)[14]	1a 9=8 6=7 4 (14) [14]	2c 8=5 6=7 2 (14)[14]	2c 9=8 7=10 4 (12)[11]
2.60.20	4	4iau	A: 80-162	sheet A: 2=1=3=6 sheet B: 7=4=5	2d* 1=3 7=4 3+2 (10)[11]	2a 3=6 7=4 3+2(9)[9]	2d 3=6 4=5 2 (8) [8]	—
2.60.30	1	1g6e	A:1-87	sheet A: 1=3=2=5=8 sheet B: 4=9=6=7	2c* 1=3 4=9 1 (7)[8]	2d 5=8 4=9 2 (7) [8]	2a 5=8 9=6 5(12)[14]	2d 5=8 6=7 3(11) [13]
2.60.34	3	4f01	B:382-506	sheet A: 5=4=1=2 sheet B: 8=7=6=3 No SubS for strands # 2 and 3	1b 5=4 7=6 6+2(15) [15]	2d 5=4 6=3 4+1(13)[15]	—	—
2.60.40.	318	1dr9	A:1-105	sheet A: 1=9=8=3=4=5 sheet B: 2=7=6 No SubS for strands # 1 and 2	1a 4=5 7=6 6 (15)[10]	2a 8=3 2=7 7(18)[15]	—	—

2.60.60	5	1rrh	A:8-167	sheet A: 4=5=1=7=8 sheet B: 3=2=6=9	1a 4=5 3=2 4 (14)[12]	2a 5=1 2=6 6+1(19)[18]	2d 7=8 6=9 6+1(15)[13]	—
2.60.90	5	1knb	A:182-365	sheet A: 10=3=2=1=5=6 sheet B: 7=8=9=4 strands #3 and 4 are parallel No SubS for strands # 4 and 5	2c 10=3 9=4 6(17)[14]	—	—	—
2.60.98.	6	1svb	A:1-51, 135-192	sheet A: 1=3=4=5=6 sheet B: 2=9=8=7 No SubS for strands # 1 and 2 strands #1 and 3 are parallel	1a 5=6 8=7 3 +1 (13)[13]	2a* 1=3 2=9 4 + 1 (14) [14]	—	—
2.60.110	1	2vhk	A:1-207	sheet A: 4=1=11=8=9 sheet B: 3=2=5=6=7=10	2d 4=1 3=2 4(13)[13]	2a 4=1 2=5 6(14)[14]	2a 11=8 7=10 2(6)[7]	2d 8=9 7=10 3(8)[10]
2.60.120	127	3HIF	A:7-130	sheet A: 1=8=3=6 sheet B: 2=7=4=5	2 d 1=8 2=7 3+2(8)[7]	2a 8=3 2=7 5(16)[12]	2a 3=6 7=4 6(15)[10]	2d 3=6 4=5 7(17)[10]
2.60.130	7	1dlm	A:3-311	sheet A: 1=5=4=7=8=9 sheet B: 2=6=3=11=10	2b 1=5 2=6 2 (9)[10]	2d 5=4 6=3 2(14)[15]	2a 4=7 6=3 3(16)[16]	1a 8=9 11=10 3(12)[9]
2.60.169	1	2bpa	1: 1-420	sheet A :1=8=3=6 sheet B: 2=7=4=5	2d 1=8 2=7 3(22)[23]	2a 8=3 2=7 4+1(23)[24]	2d 3=6 4=5 7+1(26)[24]	2a 3=6 7=4 5+1(25)[24]

2.60.175	2	4mby	H:25-300	sheet A: 1=9=3=6 sheet B: 2=7=4=5 sheet B: 8=7 No SubS for strands # 1 and 2	2d 3=6 4=5 5(15)[16]	2a 3=6 7=4 6(18)[16]	1b* 1=9 8=7 4(13)[14]	2d 3=6 2=7 5(16)[14]
2.60.200.	6	4r9p	A:27-236	sheet A: 2=1=10=9=7 sheet B: 4=3=5=6=8 strands #3 and 4 are parallel	1a 2=1 4=3 6 (17)[13]	2a 9=7 6=8 5 (15)[12]	—	—
2.60.210	1	1lb4	A:348-505	sheet A: 1=8=5=6 sheet B: 2=3=4=7 No SubS for strands # 1 and 2	1b 5=6 3=4 4 (19)[18]	2d 5=6 4=7 4 (17)[16]	2a 8=5 4=7 7 + 1 (18) [16]	—
2.60.220	6	1hn0	A:900-1020	sheet A: 1=2=3=6=7=12=9 sheet B: 4=5=8=11=10	2d 3=6 4=5 4(11)[12]	2d 6=7 5=8 3(13)[13]	2a 12=9 8=11 2(9)[14]	2d 12=9 11=10 2(8)[13]
2.60.240	3	1cq3	A:1-224	sheet A: 10=9=1=6=5 sheet B: 8=7=4=3=2 strands # 7 and 8 are parallel No SubS for strands # 1 and 2	1b 10=9 8=7 5+3(17)[19]	2d 6=5 7=4 5(14)[16]	—	—
2.60.250	1	1p35	A:2-300	sheet A: 1=4=7=6 sheet B: 10=11=12=13=9=2=3=8=5	2d 1=4 2=3= 7(16)[17]	2a 4=7 8=5 8+1(18)[13]	2d 7=6 8=5 5+1(15)[13]	—
2.60.260	4	3tj8	A:1-75	sheet A: 1=5=4 sheet B: 2=6=7=3 No SubS for strands # 3 and 4 strands #1 and 5 are parallel strands #3 and 7 are parallel	2b 1=5 2=6 4+1(11) [9]	1a 5=4 6=7 5+1(15)[14]	—	—

2.60.270.	4	1gwy	A:1-175	sheet A: 1=5=2=12=11=10 sheet B: 4=3=6=7=8=9 strands #2 and 12 are parallel	2d 5=2 4=3 4+1(12)[12]	2a 5=2 3=6 8(23)[18]	1a 11=10 8=9 3+1(9)[11]	—
2.60.290	2	1nc7	A:0-115	sheet A: 9=1=6=3=4 sheet B: 8=7=2=5	1a* 9=1* 8=7 4+2(13)[14]	2a 1=6 7=2 6+1(17)[17]	2d 1=6 2=5 7+2(20)[18]	2d 3=4 2=5 5+2(15)[15]
2.60.300	1	2apn	A: 9-104	sheet A: 1=6=7 sheet B: 3=2=5=4 strands # 1 and 6 are parallel strands # 2 and 5 are parallel	2c 1=6 2=5 4 (11) [11]	1a 6=7 5=4 4 (10) [11]	—	—
2.60.310	2	1js8	B:2787-2892	sheet A: 7=1=4 sheet B: 6=5=2=3	1a 7=1 6=5 4 (13) [11]	2a 1=4 5=2 7+2 (19) [16]	2d 1=4 2=3 7 (17) [14]	—
2.60.320	3	3ld7	A:39-125	sheet A: 2=1=7=6 sheet B: 3=4=5	1a 2=1 3=4 4 (15) [15]	1a 7=6 4=5 4+2 (14) [15]	—	—
2.60.330	1	1n7v	A: 43-66 A: 321-419	sheet A: 1=6=7=8=9 sheet B: 5=2=3=4 strands # 1, 2, 6 are parallel	2c 1=6 5=2 3 (9) [9]	—	—	—
2.60.340	1	1n80	A:12-87, 246-334	sheet A : 7=5=1=2=6 sheet B: 8=4=3	1a 1=2 4=3 4(14)[12]	2d 7=5 8=4 5(15)[16]	—	—

2.60.350	1	1x0c	A: 18-189	sheet A: 4=5 sheet A: 1=5=11=10=7 sheet B: 3=2=6=9=8	2b 1=5 2=6 4(12)[14]	1a 4=5 3=2 3+1(8)[8]	2a 10=7 6=9 5(12)[13]	2d 10=7 9=8 5(12)[11]
2.60.370	1	1so9	A:21-151	sheet A: 3=1=7=5 sheet B: 2=4=6 No SubS for strands # 2 and 3	2a 3=1 2=4 4+2(15)[15]	2a 7=5 4=6 7+2(19)[17]	—	—
2.60.390	1	1tg7	A: 577-665	sheet A: 1=4=8=7 sheet B: 2=3=5=6 No SubS for strands # 4 and 5	2d 1=4 2=3 6+1(14)[13]	1a 8=7 5=6 1(5)[6]	—	—
2.60.410	1	1hd8	A:263-356	sheet A: 4=1 sheet B: 5=7=8=3=2=6 No SubS for strands # 4 and 5	2d 4=1 3=2 3(15)[15]	2a 4=1 8=3 4(14)[12]	—	—
2.60.420	1	1h54	A:310-315, 685-753	sheet A: 1=4=5=6 sheet B: 2=3=7=8	2d 1=4 2=3 4(11)[12]	1b 5=6 7=8 5+2(15)[12]		
2.60.430	1	2p84	A:1-62	sheet A: 2=1=5 sheet B: 3=4	1a 2=1 3=4 2(9)[11]	1a 1=5 3=4 2(10)[10]	—	—
2.60.440	1	2oez	A:1-11, 179-245	sheet A: 1=4=7=2 sheet B: 5=6=3	2d 4=7 5=6 7(20)[16]	2a 4=7 6=3 5+1(16)[14]	2d 7=2 6=3 3+1(15)[14]	—
2.60.450	2	2r19	A:28-164	sheet A: 1=4=5=8=9=12=13 sheet B: 2=3=6=7=10=11=14=15	2d 1=4 2=3 2(10)[13]	2d 5=8 6=7 3+1(13)[13]	2d 9=12 10=11 3(11)[12]	1b 12=13 14=15 3(11)[12]

2.60.470	1	2qts	A: 74-96, A: 165-225	sheet A: 12=1 sheet A: 11=10=12=7=3=4 sheet B: 9=8=2=6=5 No SubS for strands # 1 and 2	1b 11=10 9=8 4 (19)[20]	2a 7=3 2=6 6(16)[13]	1a 3=4 6=5 4(12)[12]	2d 7=3 8=2 5(16)[13]
2.60.480	1	3g74	A:0-90	sheet A: 3=1=5 sheet B: 4=6=2 strands #1 and 5 are parallel strands #2 and 6 are parallel	2d 3=1 4=6 6+1(14)[13]	2a 1=5 6=2 4(14)[13]	2a* 3=1 6=2 6(15)[13]	
2.60.490	1	3h9v	A: 59-332	sheet A: 5=7 sheet A: 1=5=6 sheet B: 3=4=2=11=8=9 sheet B: 11=10	2d 1=5 4=2 3(17)[19]	1b 5=6/7 8=9 7(18)[18]		
2.60.500	1	1ywm	A: 63-160	sheet A: 1=4 sheet B: 2=3=8=7=5=6 No SubS for strands # 4 and 5	2d 1=4 2=3 3 (11) [9]	—	—	—
2.60.510	2	3tcq	A: 204-308	sheet A: 2=1=6 sheet B: 3=4=5	1a 2=1 3=4 4+1(14)[12]	1a* 1=6 4=5 5(15)[13]	—	—
2.60.520	1	1zru	A:2-140	sheet A: 1=4=3=2 sheet B: 6=5=7=8	1b 4=3 6=5 7(20) [19]	—	—	—

Table 1: Sandwich domains in 42 different folds: Supersecondary structures. Substructures.

Columns: **CATH folds:** Classification of protein folds according to CATH database; Sfam: Numbers of superfamilies in the given fold; PDB code: PDB code of the structure that represents the protein structures in this fold; **Chain fragment:** Fragment of the polypeptide chain forming a sandwich-like domain; **SSS domain:** Supersecondary structure of a sandwich like domain. The order in SSS corresponds to the arrangement of the strands in structures. “=” - backbone hydrogen bond contacts between strands in a beta-sheet. Two comments for SSS are presented if 1) two consecutive strands x and x + 1 are located in different beta-sheets and

are not described by any substructure (SubS) {see, for example, structure 1occ, CATH fold 2.60.11: there are no substructure with two strands #1 and 2 in this domain} and 2) two neighboring strands in a beta-sheet are parallel {see, for example, structure 1occ the strands #1 and 5}. In the columns **SubS 1-4** are shown 1) the classification of all substructures in the domain; 2) two pairs of strands in sheets A and B that form the substructure; 3) the total number of PHRs in the substructure + if exist, the number of pairs of oppositely charged residues (for example, in structure 4f01, CATH folds 2.60.34 in SubS 1b PHR is 6 + 2 pairs of oppositely charged residues; 4) the total number of hydrophobic residues in the substructure in round brackets (in the same SubS the number is equal to 15); 5) the total number of PCRs in the substructure in square brackets [in the same substructure the number is 15].

* In this paper, the cyclic numbering of strands in SSS is adopted: the next strand after the last strands in SSS is strand #1. Thus the last and first strands in sandwich domains are considered to be consecutive. See, for example, substructure 2c in structure 1g6e CATH folds 2.60.30.

Table 2a

PDB code	sheet A strands	Characteristics Pair of strands	sequence of strands in beta - sheet A													
			1	2	3	4	5	6	7	8	9	10	11	12	13	14
2hnu	strand 1		—	—	L 11	P 12	C 13									
	strand 2	1=2: 1 (3) [3]	G 23	F 22	C 21	R 20	G 19									
	strand 3		S 25	I 26	C 27	C 28	G 29									
	strand 4	3=4: 3 (6) [5]	G 37	V 36	F 35	C 34	G 33									
1occ	strand 1		I 52	S 51	P 50	V 49	L 48	N 47	—	—						
	strand 5	4=5: 0 (4) [5]	H 94	P 93	V 92	L 91	K 90	Y 89	H 88	T 87						
	strand 4		—	—	—	E 78	A 79	Q 80	R 81	C 82						
1h8e	strand 2		T 24	Q 25	V 26	F 27	F 28	N 29	S 30	A 31						
	strand 1	1=2: 2 (6) [7]	P 23	S 22	A 21	F 20	—	T 19	F 18	S 17						
	strand 9		E 95	A 94	L 93	L 92	—	Q 91	V 90	S 89						
	strand 8	8=9: 2 (6) [7]	S 79	G 80	S 81	V 82	—	T 83	V 84	N 85						
	strand 5	5=8: 0 (6) [7]	V 59	L 58	V 57	Q 56	—	L 55	T 54	P 53						
4iau	strand 1		A 86	T 87	L 88	Y 89	K 90									
	strand 3	1=3: 2 (6) [5]	I 118	L 117	A116	S 115	S 114									
	strand 6	3=6: 2 (5) [3]	G 141	V 142	Y 143	—	—									
1g6e	strand 1		I 2	N 3	R 4	T 5	—	—	—							
	strand 3	1=3: 0 (4)[4]	N 28	A 27	F 26	C 25	L 24	T 23	D 22							
	strand 2		—	—	L 13H	E 14	I 15H	H 16	N 17							
	strand 5		—	G 45	S 44	E 43	V 42	W 41	N 40							
	strand 8	5=8: 1 (4) [5]	—	W 70	G 71	S 72	W 73	N 74	—							
4f01	strand 5		S 453	L 454	G 455	Q 456	F 457	N 458	L459							
	strand 4	5=4: 3 (7) [7]	Q 442	L 441	V 440	H 439	I 438	T 437	V 436							
	strand 1		L 397	S 398	L 399	G 400	I 401	E 402	T 403							
	strand 2		A 413	I 412	L 411	T 410	T 409	M 408	V 407							
1dr9	strand 8		T 79	Y 80	E 81	C 82	V 83	—	V 84	L 85						
	strand 3	3=8: 3 (8) [7]	E 35	K 34	Q 33	W 32	Y 31	—	I 30	R 29						
	strand 4		—	K 37	M 38	V 39	L 40	T 41	M 42	M 43						
	strand 5	4=5: 3 (7) [4]	—	—	—	W 50	I 49	N 48	M 47	D 46						

1rrh	strand 4		–	–	–	–	E 83	G 84	I 85	I 86	–	–				
	strand 5	4=5: 2 (5) [4]	W 105	E104	F 103	N 102	I 101	K 100	F 99	A98	S 97	Q 96				
	strand 1	1=5: 3+1 (10) [10]	H 10	K 11	I 12	K 13	G 14	T 15	V 16	V 17	L 18	M 19				
	strand 7		–	–	–	E 133	L 132	T 131	L 130	S 129	V 128	L 127				
	strand 8	7=8: 3 (8) [7]	–	–	–	S 140	I 141	H 142	F 143	V144	C 145	N 146				
1knb	strand 10		–	–	–	–	–	V 573	T 574	F 575	S 576	Y 577	I 578	A 579		
	strand 3	3=10: 3 (9) [7]	V 441	A 440	L 439	V 438	S 437	V 436	T 435	A 434	L 433	I 432	Q 431	S 430		
	strand 2		D 418	A 419	K 420	L 421	T 422	L 423	V 424	L 425	T 426	K 427	C 428	–		
	strand 1		–	–	–	–	–	T 403	W 402	L 401	T 400	L 399	–	–		
	strand 5		–	–	–	–	–	W 478	N 479	F 480	R 481	N 482	–	–		
	strand 6	5=6: 0 (2) [4]	–	–	–	–	–	–	G 488	E 487	T 486	L 485	–	–		
1svb	strand 1		–	–	–	D 10	F 11	V 12	T 13	G 14	T 15					
	strand 3	1=3: 1 (6) [6]	–	–	–	C 30	V 31	T 32	I 33	T 34	A 35					
	strand 4		A 47	D 46	L 45	W 44	V 43	D 42H	M 41	S 40	P 39					
	strand 5		Y 139	T 140	V 141	K 142	V 143	E 144	P 145	H 146	–					
	strand 6	5=6: 2 + 1 (5) [6]	F 165	S 164	A 163	T 162	K 161	R 160	–	–	–					
2vhk	strand 4		G 34	E 35	S 36	W 37	T 38	I 39	N 40	V 41						
	strand 1	1=4: 3 (7) [8]	R 8	N 7	V 6	I 5	E 4	F 3	T 2	A1						
	strand 11		N 198	Y 199	R 200	V 201	T 202	F 203	C 204	–						
	strand 8	8=11: 2 (6) [7]	T 117	P 116	S 115	F 114	N 113	M 112	P 111	–						
	strand 9	8=9: 2 (3) [6]	–	R 122	G 123	V 124	R 125	C 126	A 127	–						
3HIF	strand 1		C 18	H19	I 20	H 21	K 22	Y 23	P 24							
	strand 8	1=8: 3+2 (8) [7]	I 97	E 96	A95	V 94	E 93	C 92	A 91							
	strand 3	3=8: 3 (10) [7]	L 39	Y 40	Y 41	I 42	V 43	K 44	G 45							
	strand 6	3=6: 2 (6) [4]	G 71	I 70	F 69	D 68	–	–	–							
1dlm	strand 1		V 118	S 117	E 116	P 115	A 114	–	–	–						
	strand 5	1=5: 1 (4) [5]	I 183	I 182	S 181	R 180	R 179	M 178	–	–						
	strand 4	4=5: 1 (6) [6]	K 152	V 153	E 154	I 155	W 156	H 157	A 158	–						
	strand 7	4=7: 2 (8) [7]	S 230	V 229	F 228	Y 227	H 226	I 225	H 224	A 223						
	strand 8		K 236	L 237	T 238	T 239	Q 240	I 241	N 242	V 243						
	strand 9	8=9: 1 (4) [3]	–	–	–	–	V 263	V 262	L 261	–						
2bpa	strand 1		M 10	P 11	H 12	D 13	L 14	S 15	H 16	L 17	G 18	F 19	L 20	A 21	G 22	–
	strand 8	1=8: 1 (12) [13]	R 414	Y 413	V 412	T 411	V 410	N 409	F 408	K 407	V 406	Q 405	S 404	N 403	W 402	N 403
	strand 3	3=8: 2+1(13)[14]	D 39	S 40	F 41	E 42	–	M 43	D 44	A 45	V 46	G 47	A 48	L 49	R 50	L 51
	strand 6	3=6: 3+1(13)[14]	V 277	F 276	F 275	R 274	P 273	V272	S 271	H 270	K 269	Y 268	T 267	Q 266	Q 265	V 264

4mby	strand 1		A 41	I 42	T 43	Q 44	I 45	E 46	A 47	Y 48	L 49		
	strand 9	1=9: 3 (10) [9]	K 293	R 292	L 291	T 290	V 289	N 288	F 287	Y 286	R 285		
	strand 3	3=6: 2 (7) [7]	...	A 112	V 113	S 114	V 115	K 116	T 117	...			
	strand 6		—	L 246	L 245	V 244	T 243	T 242	V 241				
4r9p	strand 2		R 75	A 74	Y 73	A 72	K 71	A 70	V 69				
	strand 1	1=2: 4 (11)[7]	W 57	A 58	K 59	V 60	I 61	V 62	F 63				
	strand 10		V 226	N 225	V 224	I 223	L 222	V 221	W 220	I 219	—		
	strand 9		—	C 201	L 202	S 203	A204	V 205	A 206	F 207	V 208		
	strand 7	7=9: 3 (9)[7]	—	—	T 143	S 142	K 141	V 140	Y 139	V 138	N 137		
1lb4	strand 1		K 356	W 355	I 354	Y 353	I 352	G 351					
	strand 8		L 494	V 495	R 496	C 497	E498	V 499	S 500	S 501			
	strand 5	5=8: 4 + 1 (8) [8]	L 435	I 434	T 433	L 432	R 431	I 430	T 429	G 428			
	strand 6	5=6: 1 (7)[8]	N 445	H 446	E 447	E 448	I 449	M 450	D 451	A 452			
1hn0	strand 3		—	—	—	N 918	V 919	T 920	G 921	Y 922	A 923	F 924	Y 925
	strand 6	3=6: 3 (9) [8]	—	—	Q 949	R 948	H 947	T 946	M 945	V 944	I 943	A 942	P 941
	strand 7	6=7: 2 (8) [7]	—	—	T 952	L 953	I 954	V 955	S 956	A 957	V 958	—	—
	strand 12		L 1020	P 1019	S 1018	L 1017	K 1016	I 1015	E 1014	Q 1013	—	—	—
	strand 9	9=12: 0 (5) [6]	K 982	W 983	Q 984	S 985	A 986	D 987	—	—	—	—	—
1cq3	strand 10		E 192	V 193	K 194	D 195	G 196	F 197	K 198	Y 199	V 200	D 201	
	strand 9	9=10: 3+2 (8) [10]	G 182	I 181	R 180	V 179	S 178	I 177	E 176	L 175	N 174	K 173	
	strand 1		G 18	I 19	D 20	V 21	I 22	I 23	K 24	V 25	T 26	K 27	
	strand 6		S 99	L 98	R 97	A 96	N 95	V 94	T 93	—	—	—	
	strand 5	5=6: 1 (5) [7]	S 84	I 85	S 86	E 87	Y 88	S 89	D 90	—	—	—	
1p35	strand 1					C 2	V 3	I 4	F 5	P 6			
	strand 4	1=4: 4 (5) [5]	S 50	I 49	N 48	F 47	M 46	M 45	L 44	V 43			
	strand 7	4=7: 6 (14) [8]	Y 148	Y149	V 150	A 151	V 152	C 153	V 154	L 155			
	strand 6	6=7: 3 (11) [8]	G 108	N 107	Q 106	C 105	S 104	V 103	S 102	Y 101			
3tj8	strand 1	1=5: 3+1 (7) [5]	R 5	E 4	I 3	I 2	M 1	—	—				
	strand 5		L 49	R 48	I 47	A 46	I 45	D 44	K 43				
	strand 4	5=4: 2+1 (7) [7]	K 33	I 34	A 35	R 36	F 37	K 38	T 39				
1gwy	strand 5		K 75	R 74	G 73	S72	Y71	L 70	L 69	A 68	K 67		
	strand 2	5=2: 2 (8) [9]	R 29	K 30	I 31	A 32	V 33	G 34	I 35	D 36	N 37	E 38	S 39
	strand 12		G 165	E 166	A 167	K 168	M 169	Q 170	I 171	K 172	I 173	S 174	R 175
	strand 11		—	—	—	T 162	M 161	I 160	G 159	K 158	M 157	R 156	L 155
	strand 10	10=11: 2+1 (6) [7]	—	—	—	—	G 145	W 146	H 147	E 148	K 149	N 150	L 151

1nc7	strand 9		–	–			Y 111	W 112	E 113	E 114	G 115	–
	strand 1	9=1: 2+2 (5) [5]	G 12	D 11	P 10	F 9	F 8	W 7	K 6	R 5	A 4	–
	strand 6	1=6: 3 (8) [9]	P 78	Y 79	S 80	I 81	M 82	A 83	E 84	S 85	N 86	V 87
	strand 3	6=3: 4 +1 (11) [10]	E 47	F 46	L 45	F 44	T 43	I 42	R 41	I 40	K 39	A 38
	strand 4	3=4: 3+1 (8) [7]	–	–	–	V 52	V 53	H 54	E 55	V 56	E 57	I 58
2apn	strand 7			–	N 98	V 97	T 96	F 95	R 94			
	strand 6	6=7: 2 (4) [5]	G 81	G 82	T 83	V 84	D 85	Y 86	T 87			
	strand 1	6=1: 1 (3) [5]	L 9	T 10	F 11	T 12	D 13	A 14	–			
1js8	strand 7		–	P 2885	T 2886	V 2887	F 2888	L 2889	A 2890			
	strand 1	7=1: 3 (8) [6]	L 2800	F 2799	G 2798	A 2797	F 2796	V 2795	R 2794			
	strand 4	1=4: 4 (9) [7]	L 2843	F 2844	K 2845	Y 2846	D 2847	I 2848	T 2849			
3ld7	strand 2		K 51	V 52		I 53	R 54	E 55	I 56	P 57	L 58	
	strand 1	2=1: 3 (9) [7]	Q 48	S 47		I 46	I 45	A 44	V 43	V 42	E 41	
	strand 7	1=7: 2 (8) [8]	V 118	F 119		V 120	E 121	I 122	K 123	S 124	T 125	
1n7v	strand 1		–	–	–	–	N 43	Y 44	W 45	G 46	–	–
	strand 6	1=6: 1 (4) [4]	–	Y 354	Y 355	A 356	V 357	Y 358	K 359	T 360	D 361	G 362
	strand 7		–	S 372	A 371	I 370	F 369	C 368	T 367	A 366	G 365	G 364
	strand 8		G 376	I 377	S 378	A 379	L 380	V 381	–	Q 382	L 383	Q 384
	strand 9		L 396	S 395	Y 394	Y 393	L 392	V 391	D 390	L 389	V 388	S 387
1n80	strand 7		E 308	M 309	I 310	Y 311	M 312	E 313	N 314	R 315		
	strand 5	7=5: 2 (6) [7]	T 276	I 275	I 274	S 273	I 272	–	Q 271	R 270		
	strand 1		I 37	F 38	I 39	T 40	F 41	–	G 42	R 43		
	strand 2	1=2: 2 (8) [7]	V 81	K 80	V 79	T 78	G 77	–	M 76	M 75		
1x0c	strand 1	1=5: 2 (6) [6]	Q 27	L 28	L 29	T 30	W 31	–	–	–	–	–
	strand 4		–	–	–	–	–	–	Y 75	L 76	A 77	I 78
	strand 5	4=5: 2 (4) [4]	S 105	Y 104	L 103	F 102	S 101	T 100	W 99	A 98	Q 97	T 96
	strand 11		–	–	S 182	A 181	F 180	L 178	L 178	L 177	A 176	N 175
	strand 10	7=10: 2 (5)[5]	–	–	–	Y 152	R 153	F 154	S 155	V 156	E 157	F 158
	strand 7		–	–	–	–	–	–	R 126	I 125	V 124	V 123
1so9	strand 3		–	–	–	–	–	R 54	D 55	I 56hb	D 57	V 58
	strand 1	1=3: 2+1 (6) [7]	A 42	V 41	N 40	A 39	D 38	F 37	T 36	V 35	K 34	I 33
	strand 7		Y 145	F 144	T 143	Y 142	S 141	L 140	T 139	L 138	K 32	E 31
	strand 5	5=7: 3 (8) [7]	–	A 82	T 83	F 84	N 85	V 86	T 87			

1tg7	strand 1		I 601	V 602	K 603	A 604	G 603	—								
	strand 4	1=4: 3+1(6) [5]	V 633	V 632	E 631	I 630	P 629	T 628								
	strand 8		I 658	W 659	S 660	A 661	S 662	V 663								
	strand 7	7=8: 1 (2) [3]	D 654	V 653	K 652											
1hd8	strand 4		V 296	—	Y 297	L 298	T 299	I 300	P 301	R 302						
	strand 1	1=4: 2 (8) [8]	L 269	P 268	N 267	V 266	T 265	E 264	F 263	F 262						
1h54	strand 1		D 309	V 310	V 311	I 312	K 313	G 314	D 315							
	strand 4	1=4: 2 (6) [7]	R 712	F 711	T 710	Y 709	S 708	T 707	W 706							
	strand 5		L 719	I 720	E 721	V 722	S 723	V 724	H 725							
	strand 6	5=6: 2+2 (7) [7]	L 734	L 733	K 732	F 731	H 730	P 729	G 728							
2p84	strand 2		G 22	M 23	S 24	Y 25	A 26									
	strand 1	1=2: 2 (5) [6]	D 11	F 10	E 9	R 8	F 7	K 6								
	strand 5	1=5: 2 (6) [5]	—	I 57	V 58	M 59	M 60	S 61								
2oez	strand 4		I 199	L 200	R 201	L 202	H 203	I 204	P 205	—						
	strand 7	4=7: 4 (9) [7]	C 245	V 244	A 243	L 242	E 241	F 240	E239	V 238						
	strand 2	2=7: 2 (8) [7]	—	H 179	F 180	K 181	A 182	Q 183	I 184	A 185						
2r19	strand 1		P 35	I 36	H 37	I 38	E 39	S 40								
	strand 4	1=4: 1 (5) [6]	G 63	Q 62	T 61	V 60	I 59	V 58								
	strand 5		T 64	I 65	K 66	I 67	N 68	A 69								
	strand 8	5=8: 2 (7) [6]	M 98	Q 97	Y 96	F 95	T 94	A 93								
	strand 9		P 104	V 105	E 106	G 107	H 108	A 109								
	strand 12	9=12: 1 (5) [6]	V 132	Q 131	Q 130	L 129	Y 128	A 127								
	strand 13	12=13: 1 (4) [6]	—	S 134	N 135	I 136	K 137	G 138								
2qts	strand 11		N 367	V 368	T 369	R 370	Y 371	G 372	K 373	E 374	L 375	S 376	M 377	V 378	K 379	I 380
	strand 10	11=10: 2 (12) [14]	I 282	L 281	R 280	Q 279	E 278	Q 277	C 276	S 275	V 274	F 273	T 272	Q 271	F 270	G 269
	strand 12		—	—	—	—	—	—	F 411	F 410	I 409	D 408	L 407	V 406	L 405	I 404
	strand 7		—	—	—	—	—	—	—	G 218	L 219	E 220	I 221	M 222	L 223	—
	strand 3	7=3: 3 (8) [6]	—	—	—	—	—	—	—	R 176	F 175	F 174	C 173	S 172	L 171	—
	strand 4	3=4: 1 (5) [5]	—	—	—	—	—	—	—	—	E 178	Q 179	C 180	S 181	P 182	—
3g74	strand 3	1=3: 3 (8) [8]	V 25	A 26	K 27	L 28	Q 29	C 30	K 31	N 32						
	strand 1		D 10	M 9	K 8	I 7	Y 6	L 5	T 4	D 3						
	strand 5	1=5: 1 (7) [8]	E 80	G 79	I 78	N 77	Q 76	I 75	D 74	V 73						

3h9v	strand 1	1=5: 2 (10) [11]	V 63	L 64	S 65	S 66	V 67	T 68	T 69	K 70	V 71	K 72	G 73
	strand 5		Y 198	R 197	I 196	N 195	N 194	K 193	I 192	L 191	V 190	T 189	F 188
	strand 6	5=6: 1 (3) [5]	F 203	N 204	K 205	R 206	N 207	–	–	–	–	–	–
	strand 7	5=7: 3 (6) [4]	–	–	–	–	–	–	–	I 232	F 233	R 234	L 235
1ywm	strand 1		A 63	A 64	T 65	L 66	N 67						
	strand 4	1=4: 2 (7) [5]	E 100	L 99	V 98	I 97	L 96						
3tcq	strand 2	1=2: 1 (5) [5]	R 214	P 215	V 216	L 217	L 218						
	strand 1		F 209	S 208	L 207	G 206	P 205	R 204					
	strand 6	1=6: 2 (6) [6]	L 303	T 304	M 305	V 306	I 307	T 308					
1zru	strand 4		R 65	Y 66	F 67	E 68	L 69	L 70	N 71	E 72	T 73	V 74	A 75
	strand 3	3=4: 4 (13) [12]	A 62	I 61	I 60	S 59	T 58	N 57	T 56	Y 55	Q 54	V 53	N 52

Table 2a: Sandwich domains in 42 different folds. Sequence of strands. Characteristics of pair of strands in beta-sheet A.

Columns: **PDB code**: see the legend for this column in Table 1; **Sheet A strands**: strands that form beta-sheet A;

Characteristics Pair of strands: for pair of strands that form the substructure are presented: 1) the total number of PHR in two pairs of hydrogen-bonded strands (for example, in structure 2hnu the number of PHR is 1 for pair of strands #1 and 2); 2) the number of hydrophobic residues is shown in round brackets (for example, in structure 2hnu the number of hydrophobic residues is 3 for pair of strands #1 and 2); 3) the total number of PCR in square brackets (for example, in structure 2hnu the total number of PCR is 3 for pair of strands #1 and 2); **Sequence of strands in beta-sheets A**: The residues that make up PCRs are shown under each other. The hydrophobic residues that make up PHRs in the substructures are bolded and enlarged. PHRs in the columns with predominantly hydrophobic residues are framed. The pairs of oppositely charged residues are bolded and italicized.

Table 2b

PDB code	sheet B strands	Characteristics Pair of strands	sequence of strands in beta-sheet B														
			1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
2hnu	strand 8	7=8: 1 (4) [5]	D 82	E 81	H 80	C 79	G 78										
	strand 7		G 71	I 72	C 73	C 74	S 75										
	strand 6	5=6: 0 (2) [3]	A 69	A 68	C 67	R 66	G 65										
	strand 5		—	—	K 59	P 60	C 61										
1occ	strand 2		N 54	K 55	R 56	I 57	V 58	G 59	C 60	I 61							
	strand 3	2=3: 4 (10) [8]	K 76	H 75	L 74	W 73	F 72	W 71	I 70	V 69							
1h8e	strand 4		G 43	A 44	F 45	G 46	I 47	L 48	A 49								
	strand 3	3=4: 2 (7) [7]	T 40	P 39	V 38	D 37	V 36	Q 35	R 34								
	strand 6		G 61	L 62	V 63	V 64	V 65	H 66	A 67								
	strand 7	6=7: 2 (8) [7]	V 77	F 76	Y 75	K 74	S 73	T 72	T 71								
	strand 10	7=10: 2 (6) [4]	A 97	V 98	T 99	L 100	—	—	—								
4iau	strand 7		K 157	S 158	M 159	E 160	R 161	E 162									
	strand 4	4=7: 1+2 (4) [6]	E 127	Y 126	L 125	R 124	W 123	Q 122									
	strand 5	4=5: 0 (3) [5]	P 134	S 135	T 136	R 137	R 138	—									
1g6e	strand 4	4=9: 1 (3) [4]	—	—	—	P 33	M 32	T 31	G 30	—							
	strand 9		H 79	E 80	I 81	S 83	I 84	R 85	I 86	Y 87							
	strand 6	6=9: 4 (8) [8]	R 55	Q 54	F 53	Q 52	L 51	T 50	V 49	V 48							
	strand 7	6=7: 2 (7) [8]	R 61	L 62	E 63	T 64	I 65	T 66	L 67	Q 68							
4f01	strand 7		I 483	L 484	H 485	V 486	S 487	A 488	K 489	D 490							
	strand 6	6=7: 3 +2(8) [8]	D 479	I 478	D 477	F 476	T 475	V 474	E 473	I 472							
	strand 3	3=6: 1 +1 (6) [8]	P 419	T 420	K 421	H 422	S 423	Q 424	V 425	F 426							
1dr9	strand 2		K 9	E 10	V 11	A 12	T 13	L 14	S 15	C 16							
	strand 7	2=7: 4 (10) [8]	L 72	A 71	L 70	I 69	V 68	I 67	S 66	L 65							
	strand 6	6=7: 3 (8) [6]	—	—	R 56	T 57	I 58	F 59	D 60	I 61							
1rrh	strand 3		G 74	K 75	L 76	G 77	K 78	A 79	T 80	F 81	L 82	—					
	strand 2	2=3: 2 (9) [8]	A 65	S 64	I 63	L 62	—	Q 61	L 60	S 59	V 58	S 57					
	strand 6	2=6: 3 (9) [8]	—	G 113	A 114	F 115	—	Y 116	I 117	K 118	N 119	F 120					
	strand 9	6=9: 3 + 1 (7) [6]	—	A 163	F 162	F 161	—	I 160	R 159	D 158	—	—					

1knb	strand 4	Q 453	S 454	A 455	H 456	L 457	I 458	I 459			
	strand 9 4=9: 3 (8) [7]	W 558	D 557	W 556	S 555	F 554	S 553	M 552			
	strand 8	V 530	T 531	L 532	T 533	I 534	T 535	L 536			
	strand 7 7=8: 2 (7) [7]	V 520	Q 519	S 518	V 517	I 516	N 515	S 514			
1svb	strand 2	—	—	T 19	R 20	V 21	T 22	L 23	V 24	L 25	E 26
	strand 9 2=9: 3 +1 (8) [8]	K 296	E 295	L 294	G 293	V 292	E 291	C 290	T 289	V288	H 287
	strand 8	G 180	Y 179	V 182	S 183	L 184	L 185	C 186	R 187	V 188	—
	strand 7 7=8: 1 (8) [7]	M 176	T 175	L 174	I 173	T 172	K 171	E 170	—	—	—
2vhk	strand 3	—	—	—	—	G 27	G 28	R 29	Q 30	L 31	
	strand 2 2=3: 1 (6) [5]	—	—	K 19	S 18	A 17	A 16	A 15	W 14	V 13	
	strand 5 2=5: 3 (7) [6]	T 45	G 47	G 48	K49H	I 50	W51	A 52	R53	—	
	strand 6	L 92	S 91	F 90H	E 89	A 88H	L 87	T 86	—	—	
	strand 7	D 98	Y 99H	I 100	D 101	I 102	—	—	—	—	
	strand 10 7=10: 1 (5) [5]	C 193	T 192	V 191	T 190	T 189	—	—	—	—	
3HIF	strand 2	K 26	S 27	T 28	—	L 29	I 30	H 31			
	strand 7 2=7: 2 (6) [5]	K 89	A88	R 87	—	V86	W85	A84			
	strand 4 4=7: 4 (9) [6]	S 46	V 47	A 48	—	V 49	L 50	I 51			
	strand 5 4=5: 5 (11) [6]	Y 63	L 64	Y 63	S 62	L 61	I 60	M 59			
1dlm	strand 2	—	—	M 123	R 122	A 121	Y 120	G 119	—	—	
	strand 6 2=6: 1(5) [5]	L 196	I 195	T 194	R 193	V 192	R 191	Y 190	Q 189	G 188	
	strand 3 6=3: 1 (8) [9]	H 132	T 133	L 134	I 135	L 136	H 137	G 138	T 139	I 140	
	strand 11	P 282	F 283	A 284	E 285	M 286	V 287	F 288	D 289	L 290	
	strand 10 11=10: 2 (8)[6]	—	H 268	E 267	V 266	A 265	D 264	V 263	—	—	
2bpa	strand 2	R 26	L 27	I 28	T 29	I 30	S 31	T 32	T 33	P 34	V 35
	strand 7 2=7: 2 (10) [10]	V 289	L 288	A 287	L 286	T 285	T 285	F 284	M 283	T 282	G 281
	strand 4 4=7: 2 (12) [10]	S 62	T 63	V 64	D 65	I 66	F 67	T 68	F 59	Y 70	V 71
	strand 5 4=5: 4 (13)[10]	A 244	W 243	L 242	N 241	S 240	R 239	M 238	V 237	L 236	L 235

4mby	strand 2		L 95	K 94	I 93	V 92	A 91	V 90	S 89	—	—	—	—	—	—	—	—
	strand 8	2=7: 3 (9) [7]	—	—	—	—	—	—	—	—	—	—	—	R 281	W 280	V 279	Q 278
	strand 7	8=7: 1 (3) [5]	D 258	K 259	L 260	F 261	L 262	S 263	C 264	A 265	D 266	I 267	A 268	G 269	V 270	H 271	T 272
	strand 4	4=7: 4 (11) [9]	—	—	—	G 156	V 155	A 154	F 153	M 152	H 151	Y 150	T 149	T 148	G 147	—	—
	strand 5	4=5: 3 (8)[9]	—	—	—	T 219	R 220	Y 221	Y 222	G 223	S 224	F 225	T 226	G 227	—	—	—
4r9p	strand 4		—	—	M 91	R 92	I 93	G 94	L 95	C 96							
	strand 3	3=4: 2 (6) [6]	P 77	V 78	L 79	T 80	I 81	N 82	G 83	S 84							
	strand 5		M 122	K 121	I 120	K 119	V 118	G 117	Q 116	—							
	strand 6	6=8: 2 (7) [6]	I 128	L 129	I 130	R 131	R 132	Y 133	A 134	—							
	strand 8		L 173	K 172	V 171	I 170	K 169	E 168	—	—							
1lb4	strand 2		T 382	Y 381	F 380	G 379 P 378	S 377	H376	I 375	V 374	—	—	V 373	P 372			
	strand 3		Y 387	K 388	L 389	C 390	M 391	R 392	L 393	H 394	—	—	L 395	Q 396	L 397		
	strand 4	3=4: 3 (12) [10]	—	M 414	T 413	H 412	V 411	F 410	L 409	S 408	—	—	I 407	Y 406	N 405		
	strand 7	4=7: 3 (10) [8]	—	—	—	G 470	F471	G 472	Y 473	V 474	T 475	F 476	M 477	H 478	L 479		
1hn0	strand 4		—	—	—	P 927	A 928	S 929	I 930	—							
	strand 5	4=5: 1 (2) [4]	—	—	K 940	N 939	V 938	K 937	K936	I 935							
	strand 8	5=8: 1 (5)[6]	V 973	T 974	I 975	N 976	V 977	T 978	I 979	N 980							
	strand 11	8=11: 2 (4) [8]	S 1007	T 1006	F 1005	T 1004	L 1003	E 1002	T1001	N 1000							
	strand 10	10=11: 2 (3) [7]	—	E 991	V 992	K 993	Y 994	Q 995	V 996	S 997							
1cq3	strand 8		I 161	I 162	G 163hb	S 164	T 165	I 166	V 167	D 168	T 169						
	strand 7	7=8: 2 + 1(9) [9]	C 124	E 125	M 126	S 127	I 128	N 129	I 130	K 131	C 132						
	strand 4	4=7: 4 (9) [9]	K 78	T 77	F 76	G 75	F 74	D 73	M 72	T 71	L 70						
	strand 3		P 59	T 60	T 61	Y 62	Y 63	T 64	V 65	V 66	G 67						
	strand 2		S 47	E 46	T 45	V 44	E 43	T 42	V 41	S 40	Q 39						
1p35	strand 2		D 10	V 11	S 12H	Q 13	T 14	I 15	I 16	R 17	D 18	C 19	—	Q20	V 21		
	strand 3	3 (11) [12]	M 35	I 34	K 33	N 32	—	I 31	Y 30	V 29	L 28	E 27	—	R 26	T 25		
	strand 8		—	—	N 164	Q 165	—	V 166	L 167	S 168	F 169	E 170	E 170	Y 171	N 172		
	strand 5	2 + 1 (4) [5]	—	—	—	—	—	—	—	T 57	V 56	S 55	R 54	I 53	P 52		

3tj8	strand 2	—	—	—	V 7	G 8	N 9	L 10					
	strand 6	2=6: 1 (4) [4]	E 66	K 65	F 64	L 63	I 62	D 61	G 60				
	strand 7	6=7: 3 (8) [7]	E 69	I 70	—	I 71	A 72	V 73	N 74				
	strand 3		S 19	V 20	D 21	Y 22	Y 22	V 23	D 24				
1gwy	strand 4		E 61	F 62	V 63								
	strand 3	4=3: 2+1 (4) [3]		R 51	F 50	Y 49	A 48	N 47	L 46	A 45	T 44	W 43	
	strand 6	3=6: 6 (15) [9]	A 84	V 85	A 86	A 87	F 88	—	A 89	Y 90	Y 91	M 92	
	strand 7		V 104	S 103	F 102	M 101	V 100	—	G 99	L 98	T 97	N 96	
	strand 8		N 113	W 114	W 115	D 116	V 117	—	K 118	I 119	Y 120	S 121	
	strand 9	8=9: 1 (3) [4]	G 142	R 141	Y 140	P 139							
1nc7	strand 8		H 102	Y 103	T 104	L 105	M 106	T 107	T 108	I 109	G 110		
	strand 7	8=7: 2 (8) [9]	G 99	V 98	D 97	L 96	R 95	S 94	L 93	Q 92	M 91	V 90	V 89
	strand 2	7=2: 3 +1 (9) [8]	—	—	—	H 25	E 26	S 27	L 28	C 29	I 30	M 31	N 32
	strand 5	2=5: 2 +1 (7) [8]	—	—	—	D 69	L 68	R 67	L 66	H 65	L 64	S 63	K 62
2apn	strand 3		E 53	D 52	F 51	T 50	F 49	G 48					
	strand 2	2=5: 3 (8) [6]	L 31	K 32	L 33	R 34	V 35	Y 36					
	strand 5		V 67	Q 68	L 69	V 70	I 71	D 72					
	strand 4	5=4: 2 (6) [6]	K 64	E 63	I 62	T 61	L 60	D 59					
1js8	strand 6		H 2875	V 2876	L 2877	S 2878	N 2879						
	strand 5	6=5: 1 (5) [5]	G 2871	K 2870	I 2869	T 2868	V 2867	K 2866	I 2865	D 2864	F 2863		
	strand 2	5=2: 3 +2 (10) [9]	A 2808	D 2809	V 2810	N 2811	F 2812	D 2813	V 2814	C 2815	T 2816		
	strand 3	2=3: 3 (8) [7]	I 2829	C 2828	F 2827	T 2826	G 2825	G 2824	F 2823	T 2822	C 2821		
3ld7	strand 3		G 63	N 64	E 65	Q 66	F 67	T 68	I 69	K 70			
	strand 4	3=4: 1 (6) [8]	G 83	D 82	V 81	E 80	M 79	L 78	N 77	Y 76			
	strand 5	4=5: 2+2 (6) [7]	—	R 85	I 86	R 87	I 88	K 89	E 90	D 91			
1n7v	strand 5		—	—	—	—	—	A 353	S 352	S 351	L 350	T 349	T 348
	strand 2	5=2: 2 (5) [5]	P 49	Q 50	A 51	L 52	H 53	A 54	Q 55	V 56	S 57	N 58	F 59
	strand 3		F 331	Y 330	N 329	N 328	T 327	I 326	R 325	L324	P 323	—	—
	strand 4		—	—	—	N 339	I 340	V 341	T 342	I 343	—	—	—

1n80	strand 8		T 325	E 326	E 327	I 328	N 329	I 330	L 331	F 332	T 333
	strand 4	8=4: 3 (9) [9]	D 254	L 253	Y 252	A 251	K 250	F 249	R 248	I 247	T 246
	strand 3	4=3: 2 (6) [5]	—	—	—	—	M 85	L 86	D 87	A 88	V 89
1x0c	strand 3		—	—	Y 69	Y 70	D 71	S 72			
	strand 2	2=3: 1 +1 (4) [4]	T 62	T 61	Q 60	V 59	K 58	V 57	S 56	Y 55	
	strand 6	2=6: 2 (6) [8]	D 107	A 108	T 109	V 110	K 111	I 112	S 113	R 114	
	strand 9	6=9: 3 (7) [8]	P 146	V 145	T 144	I 143	Y 142	V 141	S 140	Q 139	
	strand 8	8=9: 3 (7) [6]	—	F 132	P 133	V 134	R 135	Y 136	D 137		
1so9	strand 2		P 46	W 47	E 48	F 49	V 50	P 51	V 52	Q 53	
	strand 4	2=4: 2 + 1 (9)[8]	L 73	N 72	K 71	A 70	R 69	Y 68	M 67	I 66	Q 65 V 64
	strand 6	4=6: 4+2 (11)[10]	G 111	E 112	E 113	M 114	E 115	M 116	P 117	V 118	V 119 F 120
1tg7	strand 2		L 607	V 608	R 609	S 610	A 611	Y 612	L 613	D 614	
	strand 3	2=3: 3 (8) [8]	D 623	A 622	Q 621	—	I 620	H 619	L 618	D 617	
	strand 5		—	—	—	—	I 644	V 643	L 642	—	
	strand 6	5=6: 0 (3) [3]	—	—	—	—	K 647	K 648	T 649	—	
1hd8	strand 2	2=3: 1 (7) [7]	—	—	—	—	—	—	F 275	A 276	S 277 E 278 P 279 V 280 W 281
	strand 3		—	—	—	—	—	V 292	G 291	L 290	S 289 A 288 R 287 D 286 S 285
	strand 8	3=8: 2 (7) [4]	I 341	E 342	Q 343	R 344	P 345	L 346	V 347	V 348	L 349 — — —
	strand 7		Q 335	F 334	N 333	I 332	T 331	V 329	V 328	Q 327	N 326 — — —
1h54	strand 2		G 688	M 689	R 690	V 691	R 692				
	strand 3	2=3: 2 (5) [5]	A 699	Y 698	H 697	L 696	Q 695				
	strand 7		V 743	D 742	I 741	T 740	L 739				
	strand 8	7=8: 3 (8) [5]	A 746	A 747	A 748	A 749	A 750				
2p84	strand 3		E 27	Q 28	Q 29	D 30	F 31				
	strand 4	3=4: 0 (4) [5]	W 38	I 37	T 36	F 35	G 34				
2oez	strand 5		G 209	V 210	Y 211	P 212	M 213	I 214	S 215	G 216	H 217
	strand 6	5=6: 3 (11) [9]	F 228	A 227	M 226	F 225	K 224	I 223	A 222	F 221	R 220 N 219
	strand 3	3=6: 1 +1 (7) [7]				G 188	F 189	F 190	Q 191	S 192	D 193 A 194

2r19	strand 2		D 41	Q 42	Q 43	S 44	L 45	D 46	M 47
	strand 3	2=3: 1 (5) [7]	G 56	T 55	F 54	T 53	V 52	V 51	N 50
	strand 6		D 70	K 71	V 72	V 73	V 74	T 75	R 76
	strand 7	6=7: 1+1 (6) [7]	G 90	Y 89	G 88	D 87	I 86	V 85	E 84
	strand 10		S 110	Q 111	M 112	H 113	Y 114	E 115	L 116
	strand 11	10=11: 2 (7) [7]	G 125	T 124	L 123	V 122	V 121	F 120	D 119
2qts	strand 14		D 139	K 140	I 141	T 142	Y 143	L 144	V 145
	strand 15	14=15: 2 (7) [6]		F 153	A 152	Q 151	M 150	K 149	Q 148
	strand 5	5=6: 3 (7) [7]	D 184	F 185	K 186	V 187	V 188	F 189	T 190
	strand 6		N 199	F 198	T 197	Y 196	C 195	K 194	G 193
	strand 2	2=6: 3 (8) [7]	A 90	V 91	T 92	F 93	C 94	N 95	L 96
	strand 8	2=8: 2 (8) [7]	H 251	I 250	Q 249	V 248	K 247	I 246	G 245
3g74	strand 9	8=9: 2 (7) [6]	—	L 262	G 263	F 264	G 265	V 266	A 267
	strand 4		V 57	I 56	Y 55	R 54	K 53		
	strand 6	4=6: 3+1 (6) [5]	C 83	V 84	V 85	E 86	F 87		
	strand 2	2=6: 3 (7) [5]	Q 11	A 12	V 13	E 14	I 15		
	strand 3		—	—	—	—	—	—	—
	strand 4		—	—	—	—	—	—	—
3h9v	strand 2	4=2: 1 (7) [8]	—	—	—	—	—	F 102	F 103
	strand 11		—	—	F 327	V 326	M 325	V 324	D 323
	strand 8	8=9: 3 (9) [9]	D 263	W 262	R 261	I 260	Q 259	V 258	G 257
	strand 9		V 274	P 275	R 276	Y 277	T 278	F 279	R 280
								M 256	V 255
								L 282	—
1ywm	strand 2		K 82	N 73	I 74	Q 75			
	strand 3	2=3: 1 (4) [4]	I 81	Y 80	A 79	N 78			
	strand 3	3=4: 3+1 (9) [7]	F 247	K 248	I 249	V 250	P 251	I 252	
	strand 4		V 263	E 262	I 261	G 260	I 259	I 258	
	strand 5	4=5: 3 (9) [7]	P 283	I 284	I 285	P 286	V 287	L 288	
	strand 6		P 96	V 97	S 98	L 99	S 100	A 101	E 102
1zru	strand 5	5=6: 3 (7) [7]	D 89	I 88	N 87	A 86	H 85	I 84	Y 83

Table 2b. Sandwich domains in 42 different folds. Sequence of strands. Characteristics of pair of strands in beta-sheet

The legend is similar to the legend of Table 2a

Table 3a

PDB code	SubS 1a	Contacts in SubS	Intersheet Contacts	Residue- residue intersheet contacts (PHR-IC)					
2hnu	sheet A: 4=3=2=1 sheet B: 5=6=7=8	3 (1) [3]	with strand (i+2=6)	—	—	—	A 68	—	
			with strand (i+1=5)	—	—	—	—	—	
			strand (i-1=3)	S 25	I 26	C 27	C 28	G 29	
			strand (i=4)	G 37	V 36	F 35	C 34	G 33	
			with strand (i+1=5)	—	—	—	—	—	
			with strand (i+2=6)	—	—	—	A 68, A 69		
1occ	sheet A: 4=5=1 sheet B: 3=2	4 (2) [6]	with strand (i+2=5)	—	—	Y 89	—	Y 89	
			with strand (i+1=4)	—	—	—	—	C 82	
			strand (i-1=2)	R 56	I 57	V 58	G 59	C 60	I 61
			strand (i=3)	L 74	W 73	F 72	W 71	I 70	V 69
			with strand (i+1=4)	—	—	—	—	—	—
			with strand (i+2=5)	Y 89, L 91	—	Y 89	—	—	—
1h8e	sheet A: 2=1=9=8=5 sheet B: 4=3=6=7=10	4 (2) [2]	with strand (i+2=9)	—	—	L 92	—	—	—
			with strand (i+1=8)	—	—	—	—	—	—
			strand (i-1=6)	G 61	L 62	V 63	V 64	V 65	H 66
			strand (i=7)	V 77	F 76	Y 75	K 74	S 73	T 72
			with strand (i+1=8)	—	—	—	—	—	—
			with strand (i+2=9)	A 94	—	—	—	—	—
1dr9	sheet A: 1=9=8=3=4=5 sheet B: 2=7=6	6 (6) [7]	with strand (i+2=7)	—	I 67	I 67	—	—	—
			with strand (i+1=6)	—	—	I 58, F 59	—	F 59, I 61	—
			strand (i-1=4)	M 38	V 39	L 40	T 41	M 42	M 43
			strand (i=5)	—	W 50	I 49	N 48	M 47	D 46
			with strand (i+1=6)	—	—	—	—	F 59	—
			with strand (i+2=7)	—	—	—	—	—	—
1rrh	sheet A: 4=5=1=7=8 sheet B: 3=2=6=9	4 (2) [8]	with strand (i+2=5)	W 105	F 103, W 105	—	I 101, F 103	—	—
			with strand (i+1=4)	—	—	—	—	—	—
			strand (i-1=2)	I 63	L 62	Q 61	L 60	S 59	V 58
			strand (i=3)	L 76	G 77	A 79	T 80	F 81	L 82
			with strand (i+1=4)	—	—	—	—	—	—
			with strand (i+2=5)	—	—	—	—	I 101	F 99, I 101

1svb	sheet A: 1=3=4=5=6 sheet B: 2=9=8=7	3 (3) [11]	with strand (i+2=8)	C 186, V 188	—	L 184, C 186	—	V 182, L 184	—
			with strand (i+1=7)	—	—	—	—	L 174, M 176	—
			strand (i-1=5)	Y 139	T 140	V 141	K 142	V 143	E 144
			strand (i=6)	F 165	S 164	A 163	T 162	K 161	R 160
			with strand (i+1=7)	—	—	—	—	—	—
1dlm	sheet A: 1=5=4=7=8=9 sheet B: 2=6=3=11=10	3 (3) [7]	with strand (i+2=8)	L 184, C 186	—	L 184	—	—	—
			with strand (i+2=11)	—	M 286, F 288	—	M 286	—	—
			with strand (i+1=10)	—	—	—	—	—	—
			strand (i-1=8)	Q 240	I 241	N 242	V 243	—	—
			strand (i=9)	V 263	V 262	L 261	—	—	—
4r9p	sheet A: 2=1=10=9=7 sheet B: 4=3=5=6=8	6 (4) [7]	with strand (i+1=10)	—	—	—	—	—	—
			with strand (i+2=11)	M 286, V 287	—	F 288	—	—	—
			with strand (i+2=11)	F 288	—	—	—	—	—
			with strand (i+2=4)	—	—	—	I 93	—	L 95
			with strand (i+1=3)	L 79	—	—	L 79, I 81	—	—
3tj8	sheet A: 1=5=4 sheet B: 2=6=7=3	5 (4) [6]	strand (i-1=1)	W 57	A 58	K 59	V 60	I 61	V 62
			strand (i=2)	R 75	A 74	Y 73	A 72	K 71	A 70
			with strand (i+1=3)	—	L 79	—	—	—	—
			with strand (i+2=4)	—	—	—	I 93	—	—
			with strand (i+2=7)	—	—	—	—	—	—
1gwy	sheet A: 1=5=2=12=11=10 sheet B: 4=3=6=7=8=9	3 (3) [9]	with strand (i+1=6)	—	—	—	—	L 63	—
			strand (i-1=4)	K 33	I 34	A 35	R 36	F 37	K 38
			strand (i=5)	L 49	R 48	I 47	A 46	I 45	D 44
			with strand (i+1=6)	—	—	L 63	—	L 63, F 64	—
			with strand (i+2=7)	—	—	—	—	I 71	—
1gwy	sheet A: 1=5=2=12=11=10 sheet B: 4=3=6=7=8=9	3 (3) [9]	with strand (i+2=11)	M 161	M 157, I 160, M 161	—	M 157	—	L 155
			with strand (i+1=10)	—	—	—	L 151	—	L 151
			strand (i-1=8)	W 114	W 115	D 116	V 117	K 118	I 119
			strand (i=9)	R 141	Y 140	P 139	—	—	—
			with strand (i+1=10)	—	—	—	—	—	—
1gwy	sheet A: 1=5=2=12=11=10 sheet B: 4=3=6=7=8=9	3 (3) [9]	with strand (i+2=11)	—	M 157	—	—	—	—
			with strand (i+2=11)	—	—	—	—	—	—
			with strand (i+2=11)	—	—	—	—	—	—
			with strand (i+2=11)	—	—	—	—	—	—
			with strand (i+2=11)	—	—	—	—	—	—

1nc7	sheet A: 9=1=6=3=4 sheet B: 8=7=2=5	4 (1) [8]	with strand (i+2=1)	—	F 9	—	W 7, F 9	W 7	A4, W7
			with strand (i+1=9)	—	—	—	—	—	—
			strand (i-1=7)	S 94	L 93	Q 92	M 91	V 90	V 89
			strand (i=8)	T 107	T 108	I 109	G 110	—	—
			with strand (i+1=9)	—	—	W 112	—	—	—
			with strand (i+2=1)	—	—	W 7	—	—	—
2apn	sheet A: 1=6=7 sheet B: 3=2=5=4	4 (1) [1]	with strand (i+2=7)	—	—	—	—	—	—
			with strand (i+1=6)	—	—	—	—	—	—
			strand (i-1=4)	K 64	E 63	I 62	T 61	L 60	D 59
			strand (i=5)	V 67	Q 68	L 69	V 70	I 71	D 72
			with strand (i+1=6)	—	—	V 84	—	—	—
			with strand (i+2=7)	—	—	—	—	—	—
1js8	sheet A: 7=1=4 sheet B: 6=5=2=3	4 (1) [3]	with strand (i+2=1)	—	—	—	F 2799	—	—
			with strand (i+1=7)	—	—	—	—	—	V 2887
			strand (i-1=5)	K 2870	I 2869	T 2868	V 2867	K 2866	I 2865
			strand (i=6)	V 2876	L 2877	S 2878	N 2879	—	—
			with strand (i+1=7)	—	—	—	—	—	—
			with strand (i+2=1)	—	—	—	—	—	A 2797
3ld7	sheet A: 2=1=7=6 sheet B: 3=4=5	3 (1) [8]	with strand (i+2=4)	M 79	—	—	—	—	—
			with strand (i+1=3)	F 67, I 69	—	—	—	—	—
			strand (i-1=1)	I 46	I 45	A 44	V 43	V 42	E41
			strand (i=2)	I 53	R 54	E 55	I 56	P 57	L 58
			with strand (i+1=3)	F 67, I 69	—	—	F 67	—	—
			with strand (i+2=4)	—	—	—	V 81	—	V 81
1n80	sheet A : 7=5=1=2=6 sheet B: 8=4=3	4 (3) [13]	with strand (i+2=4)	—	—	L 253	—	—	—
			with strand (i+2=4)	F 249	—	F 249, A 251	—	L 253	—
			with strand (i+1=3)	—	—	—	—	—	—
			strand (i-1=1)	I 37	F 38	I 39	T 40	F 41	G 42
			strand (i=2)	V 81	K 80	V 79	T 78	G 77	M 76
			with strand (i+1=3)	M 85, L 86	—	M 85	—	—	—
			with strand (i+2=4)	F 249, A 251	—	A 251, Y 252	—	—	—
			with strand (i+2=4)	—	—	L 253	—	—	—

			with strand (i+2=5)	—	F 102	—	—	—	A 98
	sheet A: 1=5		with strand (i+1=4)	—	—	—	—	—	—
1x0c	sheet A: 4=5=11=10=7	3 (3) [3]	strand (i-1=2)	Q 60	V 59	K 58	V 57	S 56	Y 55
	sheet B: 3=2=6=9=8		strand (i=3)	Y 69	Y 70	D 71	S 72	F 73	—
			with strand (i+1=4)	—	—	—	—	Y 75	—
			with strand (i+2=5)	—	—	—	—	—	—
			with strand (i+2=8)	V 653	—	—	—	—	—
			with strand (i+1=7)	—	—	—	—	—	—
1tg7	sheet A: 1=4=8=7	1 (1) [1]	strand (i-1=5)	I 644	V 643	L 642	—	—	—
	sheet B: 2=3=5=6		strand (i=6)	K 647	K 648	T 649	—	—	—
			with strand (i+1=7)	—	—	—	—	—	—
			with strand (i+2=8)	—	—	—	—	—	—
			with strand (i+2=4)	—	—	—	—	F 35, I 37	—
			with strand (i+1=3)	—	—	—	—	—	—
2p84	sheet A: 2=1=5	2 (1) [5]	strand (i-1=1)	D 11	F 10	E 9	R 8	F 7	—
	sheet B: 3=4		strand (i=2)	G 22	M 23	S 24	Y 25	A 26	—
			with strand (i+1=3)	—	—	—	—	—	—
			with strand (i+2=4)	—	—	—	W 38	I 37, W38	—
			with strand (i+2=6)	F 198	—	—	—	—	—
	12=1		with strand (i+1=5)	—	—	F 185	—	—	—
2qts	sheet A: 11=10=12=7=3=4	4 (2) [3]	strand (i-1=3)	F 175	F 174	C 173	S 172	L 171	—
	sheet B: 9=8=2=6=5		strand (i=4)	E 178	Q 179	C 180	S 181	P 182	—
			with strand (i+1=5)	—	—	—	—	—	—
			with strand (i+2=6)	—	—	F 198	—	—	—
			with strand (i+2=4)	—	—	I 261	—	—	—
			with strand (i+1=3)	—	—	—	—	F 247	—
3tcq	sheet A: 2=1=6	4 (3) [7]	strand (i-1=1)	R 214	P 215	V 216	L 217	L 218	—
	sheet B: 3=4=5		strand (i=2)	F 209	S 208	L 207	G 206	P 205	—
			with strand (i+1=3)	I 249	—	F 247	—	—	—
			with strand (i+2=4)	I 259, I 261	—	I 261	—	—	—

Table 3a. Intersheet contacts of hydrophobic residues in the substructures 1a

Columns: **PDB code** see the legend of Table 1; **SubS 1a**: Supersecondary structure of sandwich domains. SSS of the substructure 1a is indicated by bold and enlarged numbers. **Contacts in SubS** 1) the number of PHRs in the substructure; 2) the number of PHRs

whose residues are form intersheet contacts is in round brackets; and 3) the number of PHR-IC in the substructure is in square brackets; **Intersheet Contacts**: between residues in strands $i-1$ and i in one beta-sheet and residues of strands $i+1$ and $j+1$ in another beta sheet; **Residue-residue intersheet contacts (PHR-IC)**: For example, in the structures 1occ residue **L 74** (bolded) in strand $i=3$ forms two intersheet contacts with residues Y 89 and L 91 in strand ($i+2=5$). Residue **C 60** in strand ($i-1=2$) (bolded) forms two PHR-IC with residues C 82 ($i+1=4$) and Y 89 in strand ($i+2=5$).

Table 3b

PDB code	SubS 1b	Contacts in SubS	Intersheet Contacts	Residue- residue intersheet contacts (PHR-IC)				
1h8e	sheet A: 2=1=9=8=5 sheet B: 4=3=6=7=10	4 (1) [5]	with strand (i+2=4)	—	—	—	—	A 49
			with strand (i+2=4)	—	—	—	—	I 47, L 48
			with strand (i+1=3)	—	—	—	V 36	V 36
			strand (i-1=1)	A 21	F 20	T 19	F 18	S 17 M 16
			strand (i=2)	V 26	F 27	N 29	S 30	A 31 —
			with strand (i+1=3)	—	—	—	—	—
			with strand (i+2=4)	—	—	—	—	—
4f01	sheet A: 5=4=1=2 sheet B: 8=7=6=3	6 (5) [10]	with strand (i+2=7)	—	L 484, V 486	—	V 486, A 488	—
			with strand (i+1=6)	—	F 476	—	V 474	— I 472
			strand (i-1=4)	L 441	V 440	H 439	I 438	T 437 V 436
			strand (i=5)	L 454	G 455	Q 456	F 457	N 458 L459
			with strand (i+1=6)	—	—	—	—	— I 472
			with strand (i+2=7)	—	—	—	A 488	— A 488
4mby	sheet A: 1=9=3=6 sheet B: 8=7=4=5 2=7	4 (2) [10]	with strand (i+2=1)	I 45		I 45, A 47, L 49		L 49
			with strand (i+1=9)	V 289, L 291		F 287, V 289		F 287
			strand (i-1=7)	L 260	F 261	L 262	S 263	C 264 A 265
			strand (i=8)	—	—	—	—	—
			with strand (i+1=9)	—	—	—	—	—
			with strand (i+2=1)	—	—	—	—	—
1lb4	sheet A: 1=8=5=6 sheet B: 2=3=4=7	4 (3) [7]	with strand (i+2=6)	—	—	—	—	—
			with strand (i+1=5)	I 430	L 432	—	—	—
			strand (i-1=3)	L 389	M 391	R 392	L 393	H 394 L 395
			strand (i=4)	T 413	V 411	F 410	L 409	S 408 I 407
			with strand (i+1=5)	—	I 430, L 432	—	L 432	— I 434
			with strand (i+2=6)	—	M 450	—	—	—

1cq3	sheet A: 10=9=1=6=5 sheet B: 8=7=4=3=2	5 (5) [8]	with strand (i+2=10)	—	—	—	—	—	—
			with strand (i+1=9)	I 181	—	I 177, V 179	L 175, I 177	L 175	—
			strand (i-1=7)	C 124	E 125	M 126	I 128	I 130	K 131
			strand (i=8)	I 161	I 162	G 163	T 165	V 167	D 168
			with strand (i+1=9)	V 179, I 181	I 177	—	—	L 175	—
			with strand (i+2=10)	V 193	—	—	—	Y 199	—
1h54	sheet A: 1=4= 5=6 sheet B: 2=3= 7=8	6 (5) [9]	with strand (i+2=8)	—	A 750	—	—	—	—
			with strand (i+1=7)	—	L 739, I 741	—	—	—	—
			strand (i-1=5)	L 719	I 720	E 721	V 722	S 723	V 724
			strand (i=6)	L 734	L 733	K 732	F 731	H 730	P 729
			with strand (i+1=7)	—	L 739	—	I 741, V 743	—	—
			with strand (i+2=8)	—	A 750	—	A 748, A 750	—	—
2r19	sheet A: 1=4=5=8=9= 12=13 sheet B: 2=3=6=7=10=11= 14=15	3 (3) [8]	with strand (i+2=15)	—	—	—	M 150	—	—
			with strand (i+1=14)	—	—	—	I 141, Y 143	I 141	I 141
			strand (i-1=12)	V 132	Q 131	Q 130	L 129	Y 128	A 127
			strand (i=13)	—	S 134	N 135	I 136	K 137	G 138
			with strand (i+1=14)	—	—	—	I 141	—	—
			with strand (i+2=15)	—	—	—	M 150, A 152	—	—
2qts	12=1 sheet A: 11=10=12=7=3=4 sheet B: 9=8=2=6=5	5 (3) [7]	with strand (i+2=11)	Y 371	—	—	—	—	—
			with strand (i+1=10)	V 274, C 276	—	—	—	—	—
			strand (i-1=8)	I 250	Q 249	V 248	I 246	G 245	—
			strand (i=9)	L 262	G 263	F 264	V 266	A 267	—
			with strand (i+1=10)	—	—	V 274	—	F 270	—
			with strand (i+2=11)	—	—	L 375	—	M 377	—
3h9v	sheet A: 1= 5=6/7 sheet B: 3=4=2=11= 8=9 11=10	7 (4) [8]	with strand (i+2=9)	—	—	Y 277	—	—	—
			with strand (i+1=8)	W 262	W 262	V 258, I 260	—	—	—
			strand (i-1=5)	Y 198	I 196	I 192	L 191	V 190	—
			strands (i=6/i=7)	F 203	K 205	/	I 232	F 233	—
			with strand (i+1=8)	—	—	—	—	V 258	—
			with strand (i+2=9)	—	—	—	—	Y 277, F 279	—

1zru	sheet A: 1= 4 = 3 =2 sheet B: 6 = 5 =7=8	7 (6) [14]	with strand (i+2=6)	—	—	—	—	—
			with strand (i+1=5)	I 88	A 86	I 84	—	—
			strand (i-1=3)	A 62	I 60	V 53	N 52	L 51
			strand (i=4)	R 65	F 67	V 74	A 75	L 76
			with strand (i+1=5)	—	A 86, I 88	I 84	—	I 84
			with strand (i+2=6)	—	V 97, L 99	A 101	A 101	A 101

Table 3b. Intersheet contacts of hydrophobic residues in the substructures 1b.

The legend is similar to the legend of Table 3a

Table 4a

PDB code	SubS 2a	Contacts in SubS	Intersheet Contacts	Residue- residue intersheet contacts (PHR-IC)				
1g6e	sheet A: 1=3=2= 5=8 sheet B: 4= 9=6=7	5 (2) [3]	with strand (j+1=9)	—	—	—	—	—
			with strand (i+1=6)	—	—	—	—	—
			strand (i=5)	G 45	S 44	E 43	V 42	W 41
			strand (j=8)	W 70	G 71	S 72	W 73	N 74
			with strand (i+1=6)	—	—	—	L 51, F 53	—
			with strand (j+1=9)	—	—	—	I 81	—
1dr9	sheet A: 1=9= 8=3=4=5 sheet B: 2=7=6	6 (5) [12]	with strand (j+1=8)	—	—	—	Y 80	C 82, V 84
			with strand (i+1=3)	—	—	—	W 32	W 32
			strand (i=2)	V11	A 12	T 13	L 14	S 15 C 16
			strand (j=7)	L 70	I 69	V 68	I 67	S 66 L 65
			with strand (i+1=3)	—	—	—	W 32	I 30, W 32
			with strand (j+1=8)	—	Y 80	—	Y 80	C 82, V 84
1rrh	sheet A: 4= 5=1=7=8 sheet B: 3= 2=6=9	6 (5) [9]	with strand (j+1=6)	—	—	—	—	I 117
			with strand (i+1=2)	—	L 62	—	V 58, L 60	—
			strand (i=1)	H 10	I 12	G 14	V 16	V 17 L 18
			strand (j=5)	W 105	F 103	I 101	F 99	A98 S 97
			with strand (i+1=2)	L 62, I 63	L 60, L 62	L 60	—	—
			with strand (j+1=6)	—	—	—	—	—
1svb	sheet A: 1=3=4=5=6 sheet B: 2=9=8=7	4 (4) [11]	with strand (j+1=1)	—	V 12	—	V 12	—
			with strand (i+1=3)	—	I 33	—	V 31, I 33	V 31 C 30, V 31
			strand (i=2)	T 19	V 21	T 22	L 23	V 24 L 25
			strand (j=9)	L 294	V 292	E 291	C 290	T 289 V288
			with strand (i+1=3)	I 33, A 35	I 33	—	—	—
			with strand (j+1=1)	—	—	—	—	—

2vhk sheet A: 4=1=11=8=9 sheet B: 3=2=5=6=7=10	6 (5) [10]	with strand (j+1=5)	—	I 50	—	I 50	—	—
		with strand (i+1=2)	—	A 17	—	—	—	—
		with strand (i+1=2)	—	A 15, A 16	—	—	—	—
		strand (i=1)	V 6	I 5	E 4	F 3	T 2	A1
		strand (j=4)	S 36	W 37	T 38	I 39	N 40	V 41
		with strand (i+1=2)	—	A 15, A 16	—	A 17	—	—
		with strand (i+1=2)	—	A 17	—	A 17	—	—
3HIF sheet A: 1=8=3=6 sheet B: 2=7=4=5	5 (3) [4]	with strand (j+1=5)	—	—	—	I 50	—	—
		with strand (j+1=8)	—	—	—	C 92, V 94	—	—
		with strand (i+1=3)	—	—	—	Y 40	Y 40	—
		strand (i=2)	K 26	S 27	T 28	L 29	I 30	H 31
		strand (j=7)	K 89	A88	R 87	V86	W85	A84
		with strand (i+1=3)	—	—	—	—	—	—
		with strand (j+1=8)	—	C 92	—	—	—	—
1dlm sheet A: 1=5=4=7=8=9 sheet B: 2=6=3=11=10	3 (3) [6]	with strand (j+1=7)	I 225	—	I 225, Y 227	—	—	V 229
		with strand (i+1=4)	—	—	—	—	—	V 153
		strand (i=3)	L 134	I 135	L 136	H 137	G 138	I 140
		strand (j=6)	T 194	R 193	V 192	R 191	Y 190	G 188
		with strand (i+1=4)	—	—	I 155	—	V 153, I 155	—
		with strand (j+1=7)	I 225	—	—	—	Y 227	—
		with strand (j+1=8)	—	F 408	—	—	—	—
2bpa sheet A : 1=8=3=6 sheet B: 2=7=4=5	4 (1) [6]	with strand (i+1=3)	—	A 45	—	—	—	F 41
		strand (i=2)	R 26	I 30	T 32	T 33	P 34	V 35
		strand (j=7)	V 289	T 285	F 284	M 283	T 282	G 281
		with strand (i+1=3)	L 49, L 51	—	—	F 41	—	—
		with strand (j+1=8)	—	—	—	—	—	—
		with strand (j+1=7)	L 260	—	—	—	—	—
		with strand (i+1=4)	V 155	—	—	F 153, V 155	—	—
4mby sheet A: 1=9=3=6 sheet B: 2=7=4=5	6 (4) [5]	strand (i=3)	A 112	V 113	S 114	V 115	K 116	T 117
		strand (j=6)	L 246	L 245	V 244	T 243	T 242	V 241
		with strand (i+1=4)	—	V 155	—	—	—	—
		with strand (j+1=7)	—	—	—	—	—	—
		with strand (j+1=7)	—	—	—	—	—	—

4r9p	sheet A: 2=1=10= 9=7 sheet B: 4=3=5= 6=8	5 (4) [7]	with strand (j+1=9)	—	—	V 205	—	F 207	
			with strand (i+1=7)	—	—	V 140	—	V 138	
			strand (i=6)	I 128	L 129	I 130	Y 133	A 134	
			strand (j=8)	L 173	K 172	V 171	E 168	S 167	
			with strand (i+1=7)	V 140	—	—	—	—	
			with strand (j+1=9)	A 204, V 205	—	—	—	—	
1lb4	sheet A: 1= 8=5=6 sheet B: 2=3= 4=7	7 (6) [12]	with strand (j+1=8)	C 497	—	V 495	—	—	
			with strand (i+1=5)	I 430, L 432	—	L 432	—	I 434	
			strand (i=4)	V 411	F 410	L 409	—	I 407	
			strand (j=7)	F471	G 472	Y 473	F 476	M 477	
			with strand (i+1=5)	—	—	L 432	L 432, I 434	I 434	
			with strand (j+1=8)	—	—	—	V 495	—	
1hn0	sheet A: 1=2=3=6=7= 12=9 sheet B: 4=5= 8=11=10	2 (2) [4]	with strand (j+1=12)	—	—	—	—	L 1017	
			with strand (i+1=9)	—	—	—	—	—	
			strand (i=8)	I 975	N 976	V 977	T 978	I 979	
			strand (j=11)	F 1005	T 1004	L 1003	E 1002	T1001	
			with strand (i+1=9)	—	—	—	—	—	
			with strand (j+1=12)	I 1015	—	I 1015, L 1017	—	—	
1p35	sheet A: 1= 4=7=6 sheet B: 10=11=12=13=9=2=3= 8=5	8 (6) [10]	with strand (j+1=8)	F 169, Y 171	—	L 167, F 169	—	L 167	
			with strand (i+1=5)	I 53	—	—	—	—	
			strand (i=4)	I 49	N 48	F 47	M 46	M 45	
			strand (j=7)	Y149	V 150	A 151	V 152	C 153	
			with strand (i+1=5)	—	—	I 53	—	—	
			with strand (j+1=8)	—	—	F 169	—	L 167, F 169	
1gwy	sheet A: 1= 5=2=12=11=10 sheet B: 4= 3=6=7=8=9	8 (5) [11]	with strand (j+1=6)	A 84	—	F 88	—	F 88, Y 90	
			with strand (i+1=3)	—	—	—	—	W 43	
			strand (i=2)	I 31	A 32	V 33	G 34	I 35	
			strand (j=5)	G 73	S72	Y71	L 70	L 69	
			with strand (i+1=3)	—	—	A 48, F 50	—	W 43	
			with strand (j+1=6)	—	—	F 88	—	F 88, Y 90	

1nc7	sheet A: 9= 1 =6=3=4 sheet B: 8= 7 = 2 =5	6 (5) [13]	with strand (j+1=7)	—	—	M 91	—	—	—
			with strand (j+1=7)	M 91, L 93	—	V 89, V 90			V 89
			with strand (i+1=2)	L 28	—	—	—	—	—
			strand (i=1)	F 9	F 8	W 7	K 6	R 5	A 4
			strand (j=6)	I 81	M 82	A 83	E 84	S 85	N 86
			with strand (i+1=2)	L 28	—	L 28	—	—	—
			with strand (j+1=7)	L 93	—	M 91	—	M 91	—
1js8	sheet A: 7= 1 =4 sheet B: 6= 5 = 2 =3	7 (6) [11]	with strand (j+1=5)	—	I 2865, V 2867	—	—	F 2863	—
			with strand (i+1=2)	—	V 2810, F 2812	—	F 2812	—	—
			strand (i=1)	L 2800	F 2799	G 2798	A 2797	F 2796	V 2795
			strand (j=4)	L 2843	F 2844	K 2845	Y 2846	D 2847	I 2848
			with strand (i+1=2)	—	—	—	F 2812	—	F 2812, 2814
			with strand (j+1=5)	—	—	—	—	—	F 2863, I 2865
1x0c	4=5 sheet A: 1=5=11= 10 =7 sheet B: 3=2= 6 = 9 =8	5 (4) [12]	with strand (j+1=10)	—	—	F 154	—	V 156, F 158	
			with strand (i+1=7)	—	—	—	—	—	
			strand (i=6)	A 108	T 109	V 110	K 111	I 112	
			strand (j=9)	V 145	T 144	I 143	Y 142	V 141	
			with strand (i+1=7)	—	—	V 123, I 125	—	V 123	
			with strand (j+1=10)	Y 152, F 154	—	F 154, V 156	—	V 156, F 158	
1so9	sheet A: 3=1= 7 =5 sheet B: 2= 4 =6	7 (7) [8]	with strand (j+1=7)	F 144	—	L 140, Y 142	—	—	
			with strand (i+1=5)	—	—	—	—	—	
			strand (i=4)	A 70	R 69	Y 68	I 66	Q 65	V 64
			strand (j=6)	M 114	E 115	M 116	V 118	V 119	F 120
			with strand (i+1=5)	—	—	—	—	—	V 86
			with strand (j+1=7)	—	—	—	L 140, Y 142		L 138, L 140
1hd8	sheet A: 4= 1 sheet B: 5=7= 8 =3=2=6	3 (3) [4]	with strand (j+1=1)	—	—	—	—	L 269	
			with strand (i+1=4)	—	—	—	—	V 296	
			strand (i=3)	—	—	—	—	V 292	G 291
			strand (j=8)	I 341	E 342	Q 343	R 344	L 346	V 347
			with strand (i+1=4)	L 298, I 300	—	—	—	—	
			with strand (j+1=1)	—	—	—	—	—	

2oez	sheet A: 1= 4 = 7 =2 sheet B: 5= 6 = 3	5 (4) [14]	with strand (j+1=7)	—	—	F 240, L 242	—	V 244
			with strand (i+1=4)	—	—	—	—	
			strand (i=3)	G 188	F 189	F 190	Q 191	A 194
			strand (j=6)	F 225	K 224	I 223	A 222	F 221
			with strand (i+1=4)	L 202, I 204	—	L 200, L 202	—	L 200
			with strand (j+1=7)	V 238, F 240	—	F 240, L 242	—	L 242, 244
2qts	sheet A: 11=10=12= 7 = 3 =4 sheet B: 9=8= 2 = 6 =5	6 (5) [7]	with strand (j+1=7)	—	L 219, I 221	—	I 221, L 223	—
			with strand (i+1=3)	—	—	—	—	—
			strand (i=2)	A 90	V 91	T 92	F 93	C 94
			strand (j=6)	N 199	F 198	T 197	Y 196	C 195
			with strand (i+1=3)	—	C 173, 175	—	—	—
			with strand (j+1=7)	—	L 219	—	—	—
3g74	sheet A: 3 =1=5 sheet B: 4= 6 = 2	6 (1) [3]	with strand (j+1=1)	—	—	—	—	—
			with strand (i+1=3)	—	—	V 25	—	—
			strand (i=2)	Q 11	A 12	V 13	E 14	I 15
			strand (j=6)	C 83	V84	V 85	E 86	F 87
			with strand (i+1=3)	V 25	—	V 25	—	—
			with strand (j+1=1)	—	—	—	—	—

Table 4a. Intersheet contacts of hydrophobic residues in the substructures 2a

The legend is similar to the legend of Table 3a

Table 4b

PDB code	SubS 2b	Contacts in SubS	Intersheet Contacts	Residue- residue intersheet contacts (PHR-IC)						
1dlm	sheet A: 1=5=4=7=8=9 sheet B: 2=6=3=11=10	2 (2) [7]	with strand (j+1=6)	—	—	—	—	—	—	—
			with strand (i+1=2)	Y 120	—	—	—	—	—	—
			strand (i=1)	V 118	S 117	E 116	P 115	A 114	—	—
			strand (j=5)	I 183	I 182	S 181	R 180	R 179	M 178	—
			with strand (i+1=2)	—	120, A 12	—	—	—	M 123	—
			with strand (j+1=6)	—	190, V 19	—	—	—	I 195	—
3tj8	sheet A: 1=5=4 sheet B: 2=6=7=3	4 (3) [7]	with strand (j+1=6)	—	—	L 63, F 64	—	F 64	—	—
			with strand (i+1=2)	—	—	—	—	—	—	—
			strand (i=1)	R 5	E 4	I 3	I 2	M 1	—	—
			strand (j=5)	L 49	R 48	I 47	A 46	I 45	—	—
			with strand (i+1=2)	—	—	—	—	—	—	—
			with strand (j+1=6)	L 63	—	L 63	—	L 63, F 64	—	—
1x0c	4=5 sheet A: 1=5=11=10=7 sheet B: 3=2=6=9=8	4 (3) [7]	with strand (j+1=6)	—	A 108	—	—	—	—	—
			with strand (i+1=2)	—	V 59	—	—	—	—	—
			strand (i=1)	Q 27	L 28	L 29	T 30	W 31	—	—
			strand (j=5)	S 105	Y 104	L 103	F 102	S 101	T 100	W 99
			with strand (i+1=2)	—	—	—	V 57, V 59	—	—	—
			with strand (j+1=6)	—	A 108	—	108, V 11	—	—	—

Table 4b. Intersheet contacts of hydrophobic residues in the substructures 2b

The legend is similar to the legend of Table 3a

Table 4c

PDB code	SubS 2c	Contacts in SubS	Intersheet Contacts	Residue- residue intersheet contacts (PHR-IC)					
1h8e	sheet A: 2=1=9=8=5 sheet B: 4=3=6=7=10	4 (1) [2]	with strand (j=9)	A 94	—	—	—	—	—
			with strand (i+1=8)	—	—	—	—	—	—
			strand (i=7)	V 77	F 76	Y 75	K 74	S 73	T 72
			strand (j+1=10)	A 97	V 98	T 99	L 100	—	—
			with strand (i+1=8)	—	—	—	—	—	—
			with strand (j=9)	A94	—	—	—	—	—
1g6e	sheet A: 1=3=2=5=8 sheet B: 4=9=6=7	1 (1) [6]	with strand (j=9)	—	I 86	I 84, I 86	—	—	—
			with strand (i+1=4)	—	—	—	—	—	—
			strand (i=3)	N 28	A 27	F 26	C 25	L 24	—
			strand (j+1=1)	I 2	N 3	R 4	T 5	—	—
			with strand (i+1=4)	M 32	—	—	—	—	—
			with strand (j=9)	I 84, I 86	—	—	—	—	—
1knb	sheet A: 10=3=2=1=5=6 sheet B: 4=9=8=7	6 (6) [5]	with strand (j=9)	W 556	—	W 556	—	—	—
			with strand (i+1=4)	—	—	—	—	—	—
			strand (i=3)	V 438	S 437	V 436	T 435	A 434	I 432
			strand (j+1=10)	—	—	V 573	T 574	F 575	Y 577
			with strand (i+1=4)	—	—	—	—	—	—
			with strand (j=9)	—	—	—	—	M 552, F 554	M 552
2apn	sheet A: 1=6=7 sheet B: 3=2=5=4	4 (1) [2]	with strand (j=5)	—	L 69	—	—	—	—
			with strand (i+1=2)	—	—	—	—	—	—
			strand (i=1)	T 10	F 11	T 12	D 13	A 14	—
			strand (j+1=6)	G 82	T 83	V 84	D 85	Y 86	—
			with strand (i+1=2)	—	—	—	—	—	—
			with strand (j=5)	—	—	L 69	—	—	—

1n7v	sheet A: 1=6=7=8=9 sheet B: 5=2=3=4	3 (2) [7]	with strand (j=5)	—	—	—	—	—	—
			with strand (i+1=2)	—	—	—	A 51, L 52	—	—
			strand (i=1)	—	—	N 43	Y 44	W 45	G 46
			strand (j+1=6)	Y 355	A 356	V 357	Y 358	K 359	T 360
			with strand (i+1=2)	—	A 54	—	L 52, A 54	—	—
			with strand (j=5)	A 353	A 353	—	—	—	—

Table 4c. Intersheet contacts of hydrophobic residues in the substructures 2c

The legend is similar to the legend of Table 3a

Table 4d

PDB code	SubS 2d	Contacts in SubS	Intersheet Contacts	Residue- residue intersheet contacts (PHR-IC)				
4iau	sheet A: 2= 1=3 =6 sheet B: 7=4 =5	3 (3) [5]	with strand (j=7)	M 159	—	—	—	—
			with strand (i+1=4)	W 123	—	—	—	—
			strand (i=3)	I 118	L 117	A116	S 115	S 114
			strand (j+1=1)	A 86	T 87	L 88	Y 89	K 90
			with strand (i+1=4)	W 123	—	—	—	—
			with strand (j=7)	M 159	—	M 159	—	—
1g6e	sheet A: 1=3=2= 5=8 sheet B: 4=9= 6=7	3 (3) [5]	with strand (j=7)	—	—	—	—	—
			with strand (i+1=6)	—	—	—	L 51	—
			strand (i=5)	G 45	S 44	E 43	V 42	W 41
			strand (j+1=8)	W 70	G 71	S 72	W 73	N 74
			with strand (i+1=6)	—	—	—	L 51, F 53	—
			with strand (j=7)	—	—	—	I 65, L 67	—
4f01	sheet A: 5=4 =1=2 sheet B: 8=7= 6=3	4 (3) [4]	with strand (j=5)	—	—	—	—	—
			with strand (i+1=4)	—	—	—	—	—
			strand (i=3)	H 422	S 423	Q 424	V 425	F 426
			strand (j+1=6)	F 476	T 475	V 474	E 473	I 472
			with strand (i+1=4)	F 440	—	I 438	—	V 436
			with strand (j=5)	—	—	—	—	L 459
1rrh	sheet A: 4=5=1= 7=8 sheet B: 3=2= 6=9	6 (5) [12]	with strand (j=8)	—	F 143	F 143, C 145	—	—
			with strand (i+1=7)	—	—	L 127, L 130	—	L 127
			strand (i=6)	G 113	A 114	F 115	Y 116	I 117
			strand (j+1=9)	A 163	F 162	F 161	I 160	R 159
			with strand (i+1=7)	—	—	L 127	—	—
			with strand (j=8)	I 141, F 143	F 143, V 144	V 144, C 145	—	—

2vhk	sheet A: 4=1 =11=8=9 sheet B: 3=2 =5=6=7=10	4 (2) [4]	with strand (j=3)	—	—	—	L 31	—
			with strand (i+1=2)	—	—	—	A 15, A 16, A17	—
			strand (i=1)	R 8	N 7	V 6	I 5	E 4
			strand (j+1=4)	G 34	E 35	S 36	W 37	T 38
			with strand (i+1=2)	—	—	—	A 15, A 16, A17	—
			with strand (j=3)	—	—	—	L 31	—
3hif	sheet A: 1=8= 3=6 sheet B: 2=7= 4=5	7 (3) [3]	with strand (j=5)	—	—	—	—	—
			with strand (i+1=4)	—	—	—	V 47	—
			strand (i=3)	L 39	Y 40	Y 41	I 42	V 43
			strand (j+1=6)	G 71	I 70	F 69	D 68	—
			with strand (i+1=4)	—	V 47, V 49	—	—	—
			with strand (j=5)	—	—	—	—	—
1dlm	sheet A: 1= 5=4 =7=8=9 sheet B: 2= 6=3 =11=10	2 (2) [8]	with strand (j=5)	—	—	—	—	—
			with strand (i+1=4)	—	I 155	—	—	V 153
			strand (i=3)	H 132	L 136	G 138	T 139	I 140
			strand (j+1=6)	L 196	V 192	Y 190	Q 189	G 188
			with strand (i+1=4)	A 158	I 155	V 153, I 155	—	—
			with strand (j=5)	—	I 182	I 182	—	—
2bpa	sheet A :1=8= 3=6 sheet B: 2=7= 4=5	7 (6) [13]	with strand (j=5)	V 237	—	—	—	L 242, A 244
			with strand (i+1=4)	—	—	I 66	—	V 64, I 66
			strand (i=3)	F 41	M 43	A 45	G 47	L 49
			strand (j+1=6)	F 275	V272	H 270	Y 268	Q 266
			with strand (i+1=4)	Y 70	—	—	V 64, I 66	—
			with strand (j=5)	L 235, V 237	M 238	—	—	—
4mby	sheet A: 1=9= 3=6 sheet B: 2=7= 4=5	5 (3) [5]	with strand (j=5)	—	—	—	—	—
			with strand (i+1=4)	V 155	—	—	F 153, V 155	—
			strand (i=3)	A 112	V 113	S 114	V 115	K 116
			strand (j+1=6)	L 246	L 245	V 244	T 243	T 242
			with strand (i+1=4)	—	V 155	—	—	—
			with strand (j=5)	—	Y 222	Y 222	—	—

1lb4	sheet A: 1=8= 5=6 sheet B: 2=3= 4=7	4 (4) [11]	with strand (j=6)	M 450	—	—	—	
			with strand (i+1=5)	I 430, L 432	L 432	—	I 434	
			strand (i=4)	V 411	L 409	S 408	—	I 407
			strand (j+1=7)	F471	Y 473	V 474	F 476	M 477
			with strand (i+1=5)	—	L 432	L 432	I 434	
			with strand (j=6)	M 450	I 449, M 450	—	—	
1hn0	sheet A: 1=2= 3=6 =7=12=9 sheet B: 4=5 =8=11=10	4 (3) [9]	with strand (j=5)	—	—	I 935	—	I 935, V 938
			with strand (i+1=4)	—	—	I 930	—	A 928, I 930
			strand (i=3)	T 920	G 921	Y 922	A 923	F 924
			strand (j+1=6)	T 946	M 945	V 944	I 943	A 942
			with strand (i+1=4)	—	—	—	—	—
			with strand (j=5)	—	—	I 935, V 938	—	V 938
1cq3	sheet A: 10=9=1= 6=5 sheet B: 8=7=4 =3=2	5 (5) [6]	with strand (j=6)	L 98	L 98	—	V 94, A 96, L 98	V 94
			with strand (i+1=5)	—	—	—	—	—
			strand (i=4)	F 76	F 74	D 73	M 72	L 70
			strand (j+1=7)	M 126	I 128	N 129	I 130	C 132
			with strand (i+1=5)	—	—	—	—	—
			with strand (j=6)	—	—	—	—	—
1p35	sheet A: 1=4 =7=6 sheet B: 10=11=12=13=9= 2=3 =8=5	7 (4) [9]	with strand (j=3)	—	Y 30	—	Y 30, I 34	—
			with strand (i+1=2)	—	—	—	V 11	—
			strand (i=1)	—	C 2	V 3	I 4	P 6
			strand (j+1=4)	I 49	F 47	M 46	M 45	V 43
			with strand (i+1=2)	—	—	—	—	—
			with strand (j=3)	L 28	L 28, Y 30	—	Y 30	I 34
1gwy	sheet A: 1= 5=2 =12=11=10 sheet B: 4=3 =6=7=8=9	4 (2) [7]	with strand (j=4)	—	—	—	V 63	—
			with strand (i+1=3)	—	—	—	W 43	—
			strand (i=2)	A 32	V 33	G 34	I 35	D 36
			strand (j+1=5)	S72	Y71	L 70	L 69	A 68
			with strand (i+1=3)	—	A 48, F 50	—	W 43	—
			with strand (j=4)	—	—	—	V 63	V 63

1nc7	sheet A: 9=1=6= 3=4 sheet B: 8=7= 2=5		with strand (j=4)	—	—	V 56, I 58	I 58
		5 (5) [12]	with strand (i+1=3)	—	I 42	I 40, I 42	—
			strand (i=2)	E 26	L 28	I 30	M 31
			strand (j+1=5)	L 68	L 66	L 64	S 63
			with strand (i+1=3)	I 42, F 44	I 42	—	—
1js8	sheet A: 7= 1=4 sheet B: 6=5= 2=3	7 (5) [9]	with strand (j=4)	—	V 56	V 56, I 58	—
			with strand (j=3)	F 2827	—	—	—
			with strand (i+1=2)	V 2810, F 2812	F 2812	—	—
			strand (i=1)	F 2799	A 2797	F 2796	V 2795 R 2794
			strand (j+1=4)	L 2843	Y 2846	D 2847	I 2848 T 2849
1n80	sheet A : 7=5=1=2=6 sheet B: 8=4=3	5 (5) [10]	with strand (i+1=2)	—	F 2812	—	F 2812, V 2814
			with strand (j=3)	—	F 2823, F 2827	—	—
			with strand (j=7)	—	—	—	—
			with strand (i+1=5)	I 272	—	I 274	—
			strand (i=4)	L 253	A 251	F 249	R 248 I 247
1x0c	4=5 sheet A: 1=5=11= 10=7 sheet B: 3=2=6= 9=8	5 (5) [10]	strand (j+1=8)	E 326	I 328	I 330	L 331 F 332
			with strand (i+1=5)	—	I 272	I 272, I 274	— I 274
			with strand (j=7)	—	—	Y 311	Y 311 I 310, Y 311
			with strand (j=9)	—	—	I 143	— V 141
			with strand (i+1=8)	—	—	F 132, V 134	— V 134
1tg7	sheet A: 1=4=8=7 sheet B: 2=3=5=6	5 (5) [10]	strand (i=7)	—	—	I 125	R 126 V 123
			strand (j+1=10)	Y 152	F 154	V 156	S 155 F 158
			with strand (i+1=8)	F 132	F 132	—	—
			with strand (j=9)	V 145	I 143	I 143	—
			with strand (j=3)	L 618, I 620	—	I 620	— A 622
6 (5) [11]		6 (5) [11]	with strand (i+1=2)	A 611	—	V 608	— V 608
			strand (i=1)	I 600	I 601	V 602	K 603 A 604
			strand (j+1=4)	G 634	V 633	V 632	E 631 I 630
			with strand (i+1=2)	—	—	—	—
			with strand (j=3)	—	—	L 618, I 620	— I 620, A 622

1hd8	sheet A: 4=1 sheet B: 5=7=8= 3=2 =6	3 (1) [3]	with strand (j=3)	V 292	—	—	—	—
			with strand (i+1=2)	F 275	—	—	—	—
			strand (i=1)	L 269	P 268	N 267	V 266	T 265
			strand (j+1=4)	V 296	—	Y 297	L 298	T 299
			with strand (i+1=2)	—	—	—	—	—
1h54	sheet A: 1=4 =5=6 sheet B: 2=3 =7=8	4 (2) [1]	with strand (j=3)	—	—	—	—	—
			with strand (i+1=2)	—	—	—	—	—
			strand (i=1)	V 310	V 311	I 312	K 313	G 314
			strand (j+1=4)	F 711	T 710	Y 709	S 708	T 707
			with strand (i+1=2)	—	—	—	—	—
2oez	sheet A: 1= 4=7 =2 sheet B: 5=6 =3	7 (5) [15]	with strand (j=3)	—	F 221, I 223	I 223, F 225	F 225	—
			with strand (i+1=5)	—	I 214	I 214	V 210	—
			strand (i=4)	I 199	L 200	L 202	I 204	V 238
			strand (j+1=7)	C 245	V 244	L 242	F 240	V 210
			with strand (i+1=5)	—	—	—	—	F 225
2r19	sheet A: 1=4= 5=8 =9=12=13 sheet B: 2=3= 6=7 =10=11=14=15	3 (2) [5]	with strand (j=6)	—	F 221	F 221, I 223	I 223, F 225	—
			with strand (j=7)	I 86	—	I 86	—	Y 89
			with strand (i+1=6)	—	—	V 72	—	V 72
			strand (i=5)	I 65	K 66	I 67	N 68	A 69
			strand (j+1=8)	Q 97	Y 96	F 95	T 94	A 93
2r19	sheet A: 1=4=5= 8=9 =12=13 sheet B: 2=3=6= 7=10 =11=14=15	2 (2) [5]	with strand (i+1=6)	—	—	—	—	—
			with strand (j=7)	—	—	—	—	—
			with strand (j=9)	—	—	—	—	—
			with strand (i+1=8)	—	A 93	—	—	—
			strand (i=7)	G 90	Y 89	G 88	D 87	I 86
			strand (j+1=10)	S 110	Q 111	M 112	H 113	Y 114
			with strand (i+1=8)	—	—	A 93, F 95	—	F 95
			with strand (j=9)	—	—	A 109	—	—

2qts	sheet A: 11=10=12= 7=3 =4 sheet B: 9= 8=2 =6=5	5 (5) [5]	with strand (j=7)	I 221, 219	—	I 221, L 223	—	—
			with strand (i+1=3)	—	—	—	—	—
			strand (i=2)	V 91	T 92	F 93	C 94	N 95
			strand (j+1=8)	I 250	Q 249	V 248	K 247	I 246
			with strand (i+1=3)	—	—	—	—	—
3g74	sheet A: 3=1 =5 sheet B: 4=6 =2	6 (3) [5]	with strand (j=7)	—	—	—	—	L 223
			with strand (j=6)	C 83, V 85	—	—	—	—
			with strand (i+1=4)	V 57	—	—	—	—
			strand (i=3)	V 25	A 26	K 27	L 28	Q 29
			strand (j+1=1)	D 10	M 9	K 8	I 7	Y 6
3h9v	sheet A: 1=5 =6/7 sheet B: 9=8=11= 2=4 =3 10=11	3 (1) [4]	with strand (i+1=4)	—	V 57	—	—	—
			with strand (j=6)	—	C 83	—	—	—
			with strand (j=4)	—	—	—	—	—
			with strand (i+1=2)	—	—	F 102, V 104	—	—
			strand (i=1)	T 69	K 70	V 71	K 72	G 73
1ywm	sheet A: 1=4 sheet B: 2=3 =8=7=5=6	3 (2) [4]	strand (j+1=5)	I 192	L 191	V 190	T 189	F 188
			with strand (i+1=2)	F 102	—	F 102	—	V 104
			with strand (j=4)	—	—	—	—	—
			with strand (j=3)	—	—	—	—	—
			with strand (i+1=2)	—	—	—	I 74	—
			strand (i=1)	A 63	A 64	T 65	L 66	N 67
			strand (j+1=4)	E 100	L 99	V 98	I 97	L 96
			with strand (i+1=2)	—	—	—	—	I 74
			with strand (j=3)	—	—	—	—	A 79, I 81

Table 4d. Intersheet contacts of hydrophobic residues in the substructures 2d.

The legend is similar to the legend of Table 3a

FIG. 1a

FIG. 1b

FIG. 2a

FIG. 2b

FIG. 2c

FIG. 2d

Figure 1. Conserved Substructure type 1.

Two variants of Substructures with specific arrangements of strands $i-1$, i , $i+1$, and $i+2$ (1a and 1b) are shown. Beta strands are represented by arrows and protein loops by lines. Ovals in the arrows represent residues in strands. Five positions of residues in each strand are considered. In this model, it is assumed that residues at positions 1, 3, and 5 are directed inside, while residues at positions 2 and 4 are directed outward. The 'grey positions' are occupied by hydrophobic residues.

Figure 2 Conserved Substructure type 2.

Four variants of Substructures with specific arrangements of strands i , $i+1$, j , and $j+1$ are shown in 2a, 2b, 2c, and 2d.