STRUCTURAL–FUNCTIONAL ANALYSIS
OF BIOPOLYMERS AND THEIR COMPLEXES

Role of the Structural Context in Selection of Hydrophobic Side-Chain Rotamers in a- and d-Positions of α-Helices

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Abstract—It was demonstrated for the first time that the distribution of side-chain rotamers in the a- and d-positions of α-helices of coiled-coil (cc) proteins follows a certain trend, rather then being random. For instance, most side chains adopt t rotamers in the a-positions and g^- rotamers in the d-positions of helical dimers. Vice versa, most side chains adopt g^- rotamers in the a-positions and t rotamers in the d-positions of tetramers. It was concluded that selection of the side-chain rotamers depends on the packing of α-helices and, consequently, depends on the structural context.

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INTRODUCTION

As the number of resolved protein structures is increasing in the Protein Data Bank (PDB), an increasing number of works focus on side-chain rotamers in proteins. Most works are aimed at identification of various side-chain rotamers, their classification, statistical analysis of their frequencies in proteins, and construction of rotamer databases and libraries (e.g., [1–5]). Significant differences in side-chain rotamer frequencies have been observed as dependent on the local conformation of the main chain [1–7] and the membrane environment (for membrane proteins) [8]. These studies have shown that, in proteins, side chains adopt one of the three sterically possible rotamers, which are designated as g^- ($\chi_1 = -60°$), g^+ ($\chi_1 = +60°$), and t ($\chi_1 = 180°$). In α-helical regions, the main chain imposes additional limitations on the conformational freedom of side chains, and C_β-branched side chains contained in α-helices have only one allowable conformer (Val, t; Ile and Trh, g^-), while side chains nonbranched at C_β can have either g^- or t rotamers.

However, the other factors affecting the selection of side-chain conformations in proteins are still poorly understood. We have earlier shown that a close packing of hydrophobic side chains on the surfaces of α-helices is reached owing to certain combinations of rotamers [9, 10]. The conformation of polar side chains can be selected depending on their structural environment. When a polar side chain has a partner to form a hydrogen or salt bond, one (e.g., t) conformation is selected; otherwise, the side chain adopts another conformation so that its polar moiety is accessible for water molecules [10]. In this work, we considered the role of the structural context in selection of the conformation of hydrophobic side chains with the example of α-helical leucine-zipper proteins. As a result, we observed new features of the distribution of g^- and t rotamers of side chains in hydrophobic cores of α-helical structures and revealed a dependence of the side-chain conformation on the mode of α-helix packing.

EXPERIMENTAL

Our main subject was a class of coiled-coil (cc) proteins, also known as leucine zippers. Such proteins consist of long α-helices, which are packed in a parallel or antiparallel manner to form dimers, trimers, tetramers, or, rarely, pentamers. These can be homo- or heterooligomers. In most known cc proteins, α-helices are packed with angle $\Omega \approx 20°$. In the ideal case, this angle between axes is characteristic of α-helices whose amino acid sequences have heptad repeats (abcdefg)n with a- and d-positions occupied usually by hydrophobic residues (for a review, see [11, 12]).

Such proteins are best suited for our purpose for several causes. First, many cc proteins and their model analogs have Leu in the a- and d-positions. Such an almost homogeneous set of side chains makes the

packing of α-helices nearly ideal, in contrast to heterogeneous sets, especially those with side chains dramatically differing in size. To study the selection of side-chain rotamers, our sample included only the cc proteins having the a- and d-positions occupied mainly by Leu, Phe, and Tyr residues (their side chains are most similar in size and can have two rotamers), but not proteins containing mostly Val and Ile in the a- and d-positions (see Tables 1–5). In addition, out database included homologous proteins and their model analogs that can be switched, e.g., from dimers to trimers or tetramers as a result of point mutations. This is of special importance for studying the effect of the structural context on the selection of side-chain conformations, because the same or a very close set of side chains occurs in different structural environments in such cases. Another advantage of cc proteins is that their α-helices are rather long (mostly, of 20 or more residues), which substantially reduces the marginal effects. Necessary structural information was taken from PDB (http://www.rcsb.org/pdb/). Torsion angle χ_1 was computed using the MOLMOL program [13].

RESULTS AND DISCUSSION

The packing of α-helices against each other in proteins follows two main patterns, face-to-face and side-by-side, which differ in the arrangement of hydrophobic surfaces (or clusters) [9, 10, 12]. In the case of face-to-face packing, hydrophobic clusters are between the backbones of α-helices in the contact region and form a bilayer of hydrophobic side chains. Such a packing is observed in all dimeric cc proteins with a parallel or antiparallel arrangement of α-helices and in long isolated α-helical hairpins of globular proteins (Tables 1, 2). In the case of side-by-side packing, hydrophobic clusters are combined to form a single layer of hydrophobic side chains on the surface of the double-helical structure. Such α-helix packing is observed in tetramers and pentamers of cc proteins (Tables 4, 5) and in four-helix bundles of globular proteins. In trimeric cc proteins, the packing of α-helices is most similar to side-by-side packing but shows some features of face-to-face packing (Table 3). Thus, depending on the α-helix packing, hydrophobic side chains are arranged differently relative to each other and to the backbones of the α-helices and, consequently, occur in different structural environments, which substantially affects their conformation.

Table 1 summarizes the angles χ_1 computed for all residues occupying the a- and d-positions of cc dimers whose α-helices are packed face-to-face and are parallel. Analysis of these data revealed an important feature in the distribution of rotamers of the hydrophobic side chains that are sterically allowed to adopt two conformations (Leu, Phe, Tyr, etc.). Most of the chains occur as t rotamers in the a-positions and as g⁻ rotamers in the d-positions. To illustrate, Fig. 1 shows a circular diagram of the χ_1 distribution for Leu residues occurring in the a- and d-positions of cc dimers with parallel α-helices.

Angles χ_1 computed for residues occupying the a- and d-positions in α-α-hairpins and antiparallel dimers are summarized in Table 2; their distribution is shown in Fig. 2. Although less distinct, the feature observed in this case was the same as in dimers with parallel α-helices. The side-chain conformation will be considered a t rotamer when χ_1 ranges from −150° to +150° and a g⁻ rotamer when χ_1 ranges from −50° to −100°. These criteria are more stringent than, for example, in [7], where $\chi_1 = 180 \pm 60°$ suggested t rotamers and $\chi_1 = 0$ to −120°, g⁻ rotamers. A simple calculation shows that 64% of the side chains of Leu, Phe, and Tyr occupying the a-positions in antiparallel dimers and hairpins adopt t rotamers; 19% adopt g⁻ rotamers, and 17% have sterically prohibited conformations (Fig. 2). For a comparison, 75% of Leu residues in the a-positions of dimers with parallel α-helices adopt t rotamers, 21% adopt g⁻ rotamers, and 4% have sterically prohibited conformations (Fig. 1). In the d-positions of hairpins and antiparallel dimers, 76% of Leu, Phe, and Tyr side chains adopt g⁻ rotamers, 12% adopt t rotamers, and 12% have sterically prohibited conformations (Fig. 2). In parallel dimers, virtually all Leu residues in the d-positions adopt g⁻ rotamers (Fig. 1). We think that the distribution (Fig. 2) displayed a greater number of deviations from the general trend as compared to that in Fig. 1 because the side-chain composition of antiparallel dimers and hairpins was more heterogeneous.

The distribution of side-chain rotamers in trimeric proteins substantially differed from that in dimers. As evident from Table 3 and Fig. 3, most (75%) of the a-position side chains of trimers adopt g⁻ rotamers, rather than t rotamers, as in dimers. As for the d-positions, the situation with trimers was similar to that with dimers: 63% of the residues adopt g⁻ rotamers, 25% adopt t rotamers, and 12% have sterically prohibited conformations. A similar distribution was observed for tetramers-1 (the a- and d-positions of tetramers-1 are occupied mostly by Leu, while the composition of tetramers-2 is heterogeneous): 82% of Leu residues in the A-positions adopt g⁻ rotamers, t rotamers are absent, and 18% of residues have sterically prohibited conformations (Table 4, Fig. 4). Of the five residues found in the d-positions of tetramers-1, three adopt g⁻ rotamers and two adopt t rotamers.

The rotamer distribution in tetramers-2 is opposite to that in dimers: most side chains in the a-positions adopt g⁻ rotamers, while side chains in the d-positions mostly adopt t rotamers (Table 5, Fig. 5). According to our estimates, 83% of the Leu, Phe, and Tyr residues in the a-positions of tetramers-2 adopt g⁻ rotamers, 8% adopt t rotamers, and 9% have sterically prohibited conformations. In the d-positions of tetramers-2,

Parallel dimers

a-positions
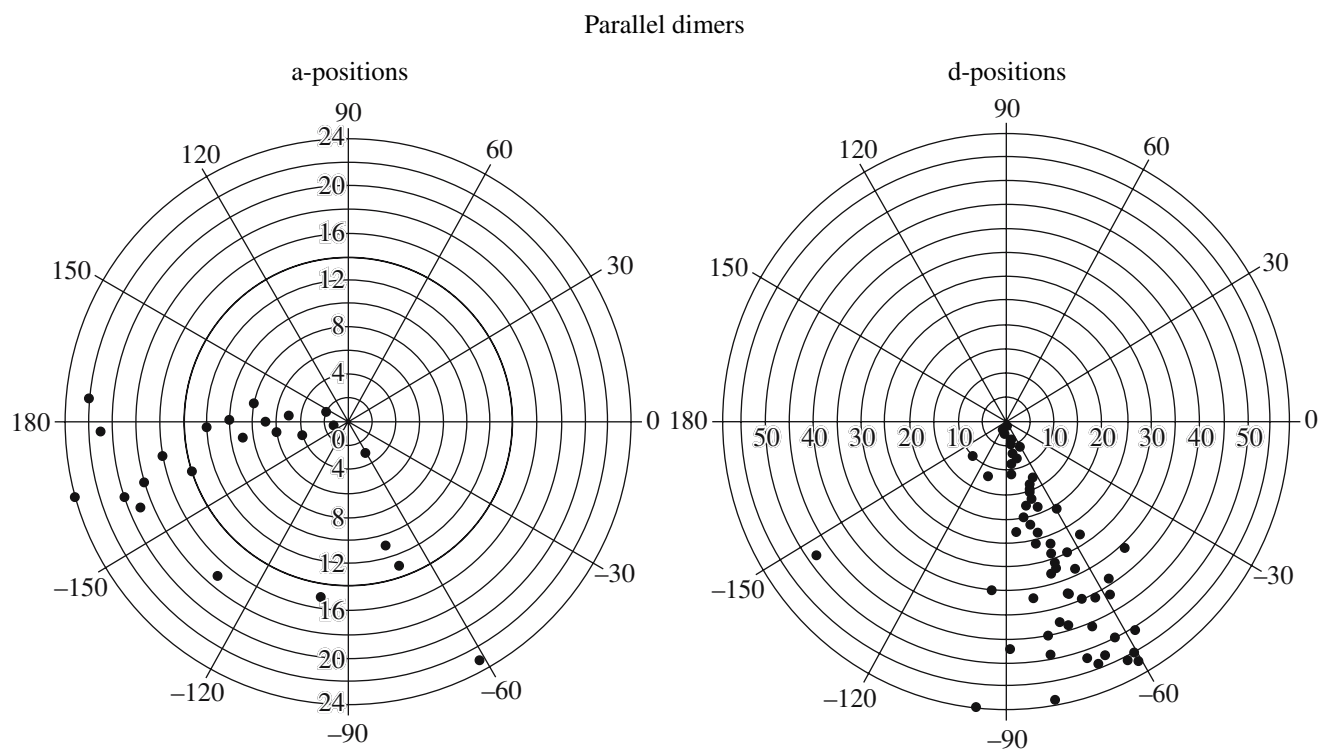
d-positions

Fig. 1. Torsion angle χ_1 distribution of Leu residues occupying the a- and d-positions in parallel cc dimers (based on Table 1). Here and in Figs. 2–5, distributions are shown as circular diagrams. The upper half-circles correspond to positive (χ_1 ranging from 0 to 180°) angles and the lower ones, to negative (χ_1 ranging from 0 to –180°) angles.

Antiparallel dimers and hairpins

a-positions
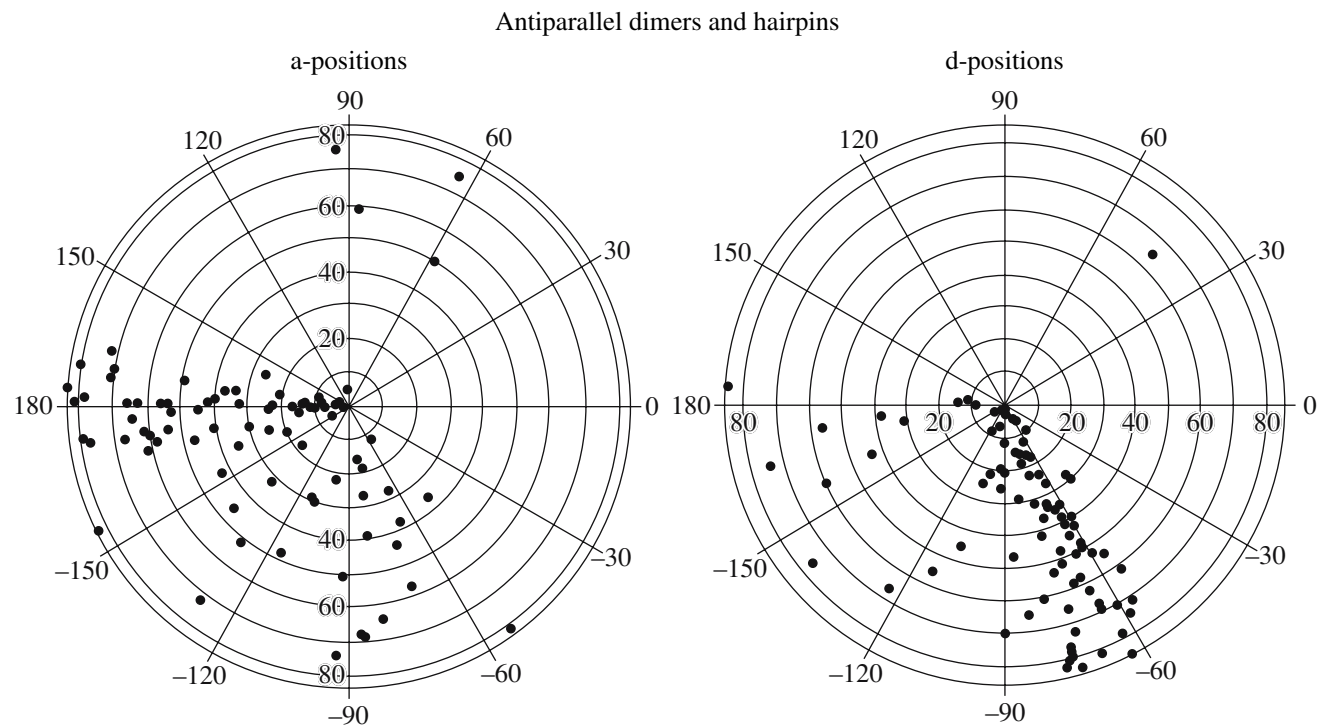
d-positions

Fig. 2. Torsion angle χ_1 distribution of Leu, Phe, and Tyr residues occupying the a- and d-positions in antiparallel cc dimers and α-helical hairpins (based on Table 2).

Trimers

a-positions
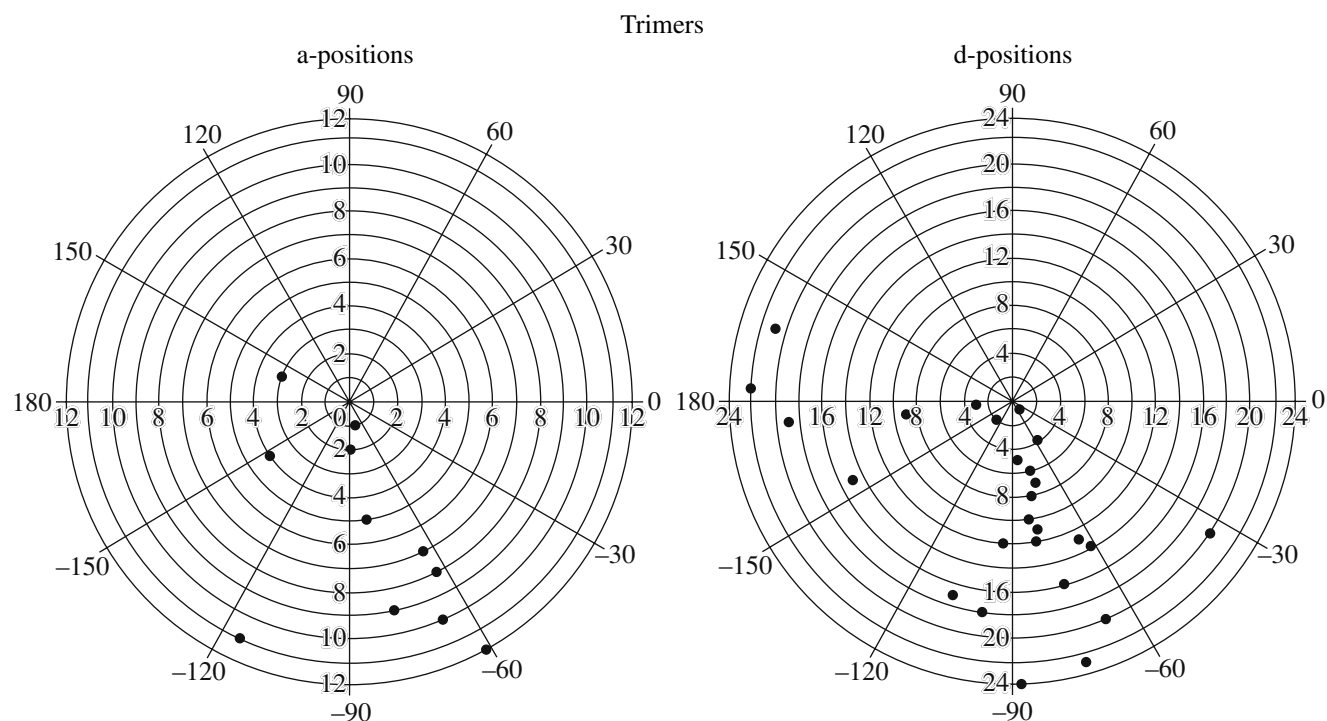
d-positions

Fig. 3. Torsion angle χ_1 distribution of Leu, Phe, and Tyr residues occupying the a- and d-positions in trimers (based on Table 3).

Tetramers-1

a-positions

d-positions

Fig. 4. Torsion angle χ_1 distribution of Leu residues occupying the a- and d-positions in tetramers-1 (based on Table 4).

Fig. 5. Torsion angle χ_1 distribution of Leu, Phe, and Tyr residues occupying the a- and d-positions in tetramers-2 (based on Table 5).

80% of residues adopt t rotamers and 20% adopt g⁻ rotamers.

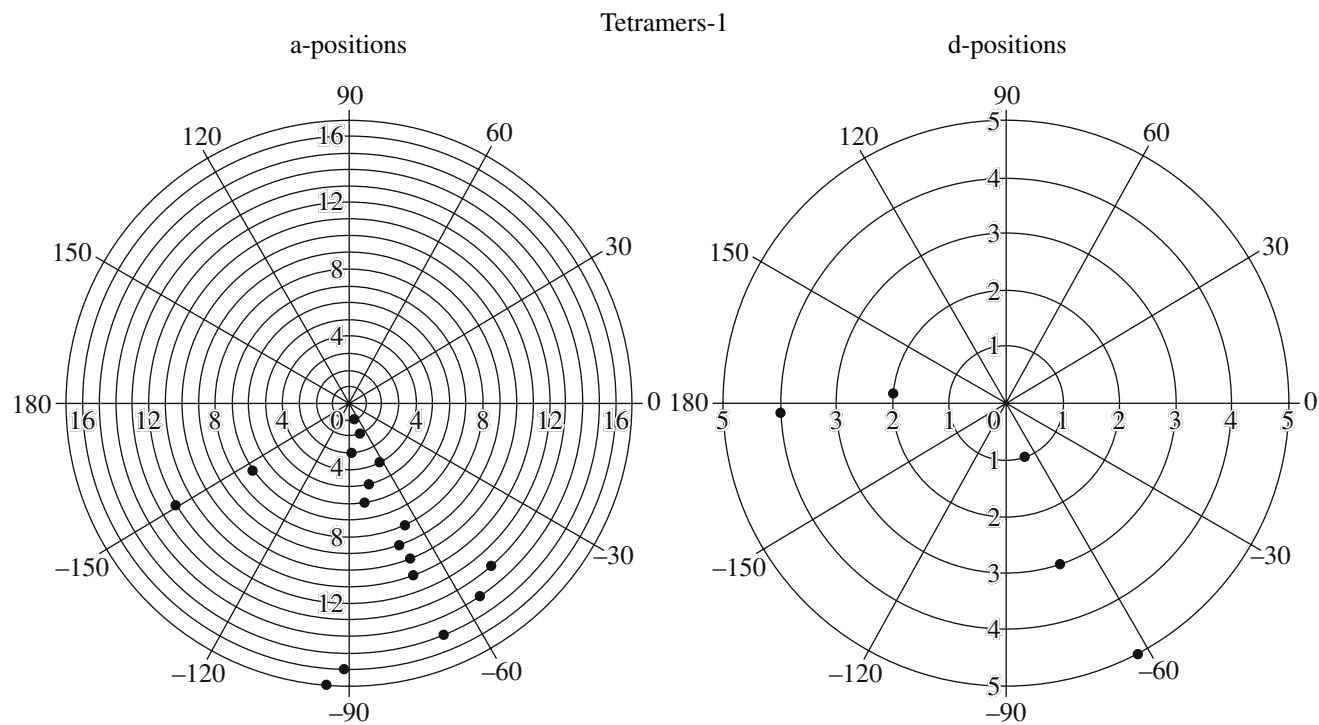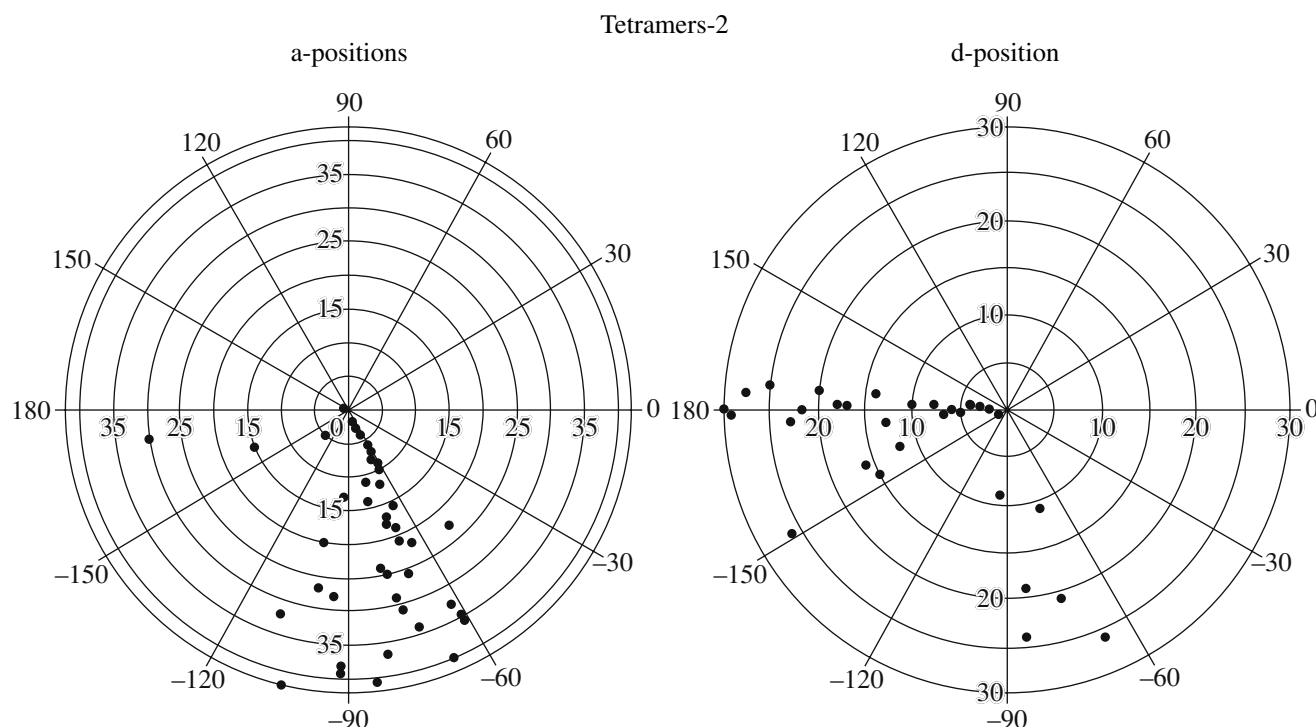Thus, a trend is distinct: the conformation of side chains changes from t to g⁻ rotamers in the a-positions and from g⁻ to t rotamers in the d-positions upon the transition from dimers to trimers and tetramers; i.e., as the α-helix packing changes from face-to-face to side-by-side. In the intermediate cases of trimers and tetramers-1, especially with a homogeneous set of side chains, g⁻ rotamers are prevalent in both a- and d-positions. In other words, the selection of side-chain rotamers in the a- and d-positions depends on the α-helix packing and, consequently, on the structural context.

The trend observed can be explained by a simple squeezing mechanism; i.e., the side chains are squeezed out of the helix–helix interface. A possible scenario is considered below with the example of dimers. Assume that dimers initially have g⁻ rotamers of side chains in the a-positions and t rotamers in the d-positions. In this case, a major part of each side chain in these positions occur in the space between the backbones of α-helices. As the a-position side chains adopt t rotamers and the d-position side chains adopt g⁻ rotamers (as observed), the centers of mass of the side chains are displaced from the helix–helix interface outwards, and the tendency to a closer packing reduces the distance between the axes of the α-helices. Thus, the interactions between helices and the tendency to a closer packing bring the axes of the α-

helices close together and displace the side chains from the between-helix space. This mechanism will be detailed elsewhere.

The trends observed in the rotamer distribution in dimers, trimers, and tetramers of cc proteins are of importance. Advantage of them can be taken in modeling protein structures and designing new structures in protein engineering. It should be noted that the side-chain rotamers can be predicted not only for Leu, Phe, and Tyr, but also for β-branched Val and Ile, because these residues each have a single sterically allowable rotamer in the vast majority of cases (as can be seen from Tables 1–5).

The observed deviations from the above trends can be explained by the effects of the following factors. Analysis showed that such deviation occur mostly at the ends of helices; i.e., marginal effects do take place. This is possibly because α-helices are diverged from each other at the ends of some oligomers and no longer affect each other. The heterogeneity of the sets of a- and d-position side chains can further contribute to the deviations. For instance, the trends are more distinct in parallel dimers, which have almost homogeneous sets of Leu residues (Fig. 1), than in antiparallel dimers, whose sets of side chains are heterogeneous (Fig. 2).

To conclude, it should be noted that similar trends in the distributions of side-chain rotamers were observed for four-helix bundles (our preliminary data)

Table 1. Angle χ_1 for residues in the **a**- and **d**-positions in dimers of cc proteins with a parallel α-helix packing*

No.	PDB ID	a	d	a	d	a	d	a	d	a	d	a	d	a	d	a	d	a	d	a	d
1	1D7M(A)		M244 −72	L248 −164	L251 −84	L255 −172	E258 −84	R262 171	L265 −73	K269 −179	L272 −89	L276 −98	L279 −69	G283 −	R286 171	L290 −162	L293 −80	L297 −178	T300 −56	N304 −61	E307 −142
		R311 169	L314 −78	L318 174	T321 −67	R325 179	L328 −85	L332 −178	A335 −	K339 −164											
2	1DH3(A)	E287 −155	L290 −103	R294 102	A297 −	R301 −136	K304 −120	V308 −26	L311 −65	V315 95	L318 −79	N322 −93	L325 −61	L329 −131	L332 −61						
3	1GD2(E)	L101 −167	L104 −92	V108 169	L111 −109	H115 169	T118 50	N122 174	L125 −95	V129 79	L132 −63	L136 −170	L139 −								
4	1ZII(A)	M2 −176	L5 −77	V9 167	L12 −65	A16 −	L19 −74	V23 171	L26 −47	V30 164	R33 −										
5	1UIX(A)	V982 171	L985 −78	K989 −72	L992 −69	L996 179	A999 −	L1003 −71	L1006 −81	E1010 −	A1013 −	K1017 162	F1020 −96	L1024 −164	E1027 −76	K1031 171	A1034 −	L1038 175			
6	1KDD(A)	V2 178	L5 −63	V9 167	L12 −70	L16 −73	L19 −74	V23 166	L26 −70	N30 −173	C33 −177										
7	1CZ7(A)	L321 157	C324 180	L328 −172	S331 −165	R335 −169	L338 −76	V342 162	L345 −57												
8	1KQL(A)	V32 171	L35 −78	N39 −82	L42 −71	V46 167	L49 −70	V53 162	L56 −67	L60 −163	Q63 −164	Y67 −165	I70 −133	L74 −158	A77 −	M81 172					
9	1S9K(D)		L165 −74	T169 56	L172 −72	K176 −178	L179 −57	I183 −66	L186 −63	K190 170											
10	1S9K(E)	R280 −83	K283 −159	I287 −53	L290 −76	V294 −175	L297 −71	N301 −89	L304 −59	A308 −	L311 −58	V315 168	L318 −63								
11	1LLM(C)	H50 159	I53 −59	L57 −180	L60 −70	V64 169	L67 −65	N71 −75	L74 −75	V78 166	L81 −71	V85 −39									
12	1CE9(A)	V3 47	L6 −83	V10 167	L13 −80	N17 −84	L20 −71	V24 165	L27 −73	V31 149	R34 −104										
13	1T6F(A)	L2 −104	A5 −	N9 −172	L12 −60	I16 −68	K19 −79	I23 −69	L26 −79	N30 −72	L33 −67	A37 −									
14	1P9I(A)	M1 −	L4 −135	L8 169	L11 −77	N15 174	L18 −71	V22 166	L25 −67	V29 163											

Note: *Here and in Tables 2–5, angle χ_1 is measured in degrees and is indicated below the corresponding residue.

Table 2. Angle χ_1 for residues in the **a**- and **d**-positions in dimers of cc proteins and α-helical hairpins with an antiparallel and face-to-face α-helix packing

No.	PDB ID	a	d	a	d	a	d	a	d	a	d	a	d	a	d	a	d
1	1A32(1)		P24 / –	I28 / –65	L31 / –88	I35 / –67	L38 / –171	L42 / –92									
2	1A32(2)		S51 / –57	L55 / 177	M58 / –73	R62 / –170	L65 / –74	L69 / –129	K72 / –177								
3	1A36(1)	M644 / –	L647 / –74	I651 / –67	K654 / –35	L658 / 173	A661 / –	L665 / –178	A668 / –	A672 / –							
	1A36(2)		T680 / –56	V684 / 179	K687 / –76	V691 / 172	L694 / –68	L698 / 179	L701 / –71	A705 / –	R708 / –60						
4	1AQT(1)	E91 / –173	A94 / –	K98 / 179	A101 / –76	I105 / –70											
	1AQT(2)	Y114 / 171	A117 / –	L121 / –173	A124 / –	L128 / –66	I131 / –73										
5	1CXZ(1)		A28 / –	Q32 / –78	L35 / –64	R39 / –76	L42 / –68	I46 / –70	E49 / –153	K53 / –112	A56 / –	R60 / –167	T63 / –90	G67 / –			
	1CXZ(2)		V73 / –152	L77 / –81	S80 / –175	L84 / –82	L87 / –62	L91 / –173	L94 / –60								
6	1DG3(1)		R539 / –175	L543 / –180	Q546 / –80	L550 / 177	K553 / –74	Q557 / –168	L560 / –74								
	1DG3(2)	S569 / 180	M572 / –77	I576 / –65	L579 / 177	M583 / –70											
7	1E79(1)	L105 / –149	A108 / –77	L112 / –65	A115 / –	L119 / –171											
	1E79(2)	R128 / –72	I131 / –41	I135 / –66	N138 / –75	V142 / –176	L145 / –65										
8	1FXK(A1)	V7 / –170	Q10 / –95	F14 / 179	L17 / –79	A21 / –	I24 / –78	K28 / –166	V31 / 78	I35 / –84	T38 / –61	L42 / –86	L45 / –90				
	1FXK(A2)		K67 / 165	T71 / –61	L74 / –74	L78 / 178	L81 / –72	E85 / 174	I88 / –69	E92 / –179	V95 / 170	L99 / –82	M102 / –	I106 / –72			
	1FXK(A3)	L7 / –176	I10 / –55	L14 / –77	Y17 / –75	V21 / 168	I24 / –65	M28 / –73	V31 / 179	I35 / –74	L38 / –79	E42 / –79	L45 / –61	Q49 / –68			
	1FXK(A4)	M94 / –66	I97 / –67	K101 / –64	L104 / –67	L108 / –153	M111 / –69	L115 / 179	L118 / –62	M122 / –71	L125 / –55	A129 / –	L132 / –57	V136 / 66			
9	1GRJ(1)	A11 / –	L14 / –122	L18 / –158	L21 / –57	R26 / 176	I29 / –72	I33 / –51	A36 / –								
	1GRJ(2)	Y48 / 179	A51 / –	Q55 / –146	C58 / –68	I62 / –68	I65 / –64	L69 / –71									

Table 2. (Contd.)

No.	PDB ID	a	d	a	d	a	d	a	d	a	d	a	d	a	d	a	d	a	d	a	d
10	1IDS(1)		G22 –	E26 -178	H29 -179	H33 -165	Y36 -63	A40 –	A43 -60	L47 -81	A50 –											
	1IDS(2)		N62 -68	L66 170	N69 -76	H73 178	H76 -72	W80 -57	L83 -57													
11	1QOJ(1)	P629 –	L632 -89	I636 -86	L639 -64																	
	1QOJ(2)	A655 –	I658 -63	L662 -100	L665 -76	F669 -177	A672 –															
12	1QSD(1)	L6 177	K9 -66	L13 180	L16 -95	E20 -173	Y23 -75	L27 -170	Q30 -76	V34 170	L37 -66											
	1QSD(2)	L48 164	Q51 -131	L55 -178	T58 -56	L62 -71	L65 -175	I69 -73	F72 -74	L76 -177	F79 176											
13	1SRY(1)	L30 -178	L33 -144	V37 172	L40 -91	L44 -179	V47 -179	R51 -163	V54 154													
	1SRY(2)		L69 -64	G73 172	L76 -103	A80 –	L83 -64	L87 -160	K90 -72	L94 179	L97 45											
14	1CII(1)		L232 -57	Q236 71	L239 -116	Q243 -165	N246 179	I250 -60	A253 –	L257 173	V260 168	L264 171	A267 –	L271 -172	A274 –	L278 178	Q281 -59					
	1CII(2)		A383 –	I387 -56	A390 –	V394 158	A397 –	L401 -172	R404 -72	Q408 -167	A411 –	L415 173	L418 -73	K422 -176	I425 -72	L429 -164	I432 -77	I436 -61	E439 172	Q443 -159	–	
	1CII(3)	R67 -67	I70 -47	D74 -90	I77 -73	K81 -73	L84 -60	Q88 -173	N91 -112	R95 -180	A98 –	L102 167	A105 –	R109 -159	D112 -76	L116 -173	L119 -141					
	1CII(4)	I129 -65	Q132 -170	L136 159	A139 –	E143 -178	F146 -63	I150 -53	Y153 -76	R157 -164	T160 -58	M164 -71	A167 –									
15	1L8D(1)	L399 -178	L402 -105	K406 173	I409 -60	R413 -176	I416 -68	I420 -77	L423 -114	I427 -70	L430 -84	I434 -77	L437 -166									
	1L8D(2)	D453 -59	R456 175	L460 -81	Y463 -69	L467 -139	S470 -58	L474 -173	L477 -112	K481 -178	L484 -73	L488 -128	I491 -147	I495 -67	L498 -59							
16	1FPO(1)	T17 55	L20 179	F24 164	L27 -72	Y31 -54	–															
	1FPO(2)	Q44 -65	A47 –	S51 -169	I54 -60	W58 152	L61 -64															

Table 2. (Contd.)

No.	PDB ID	a	d	a	d	a	d	a	d	a	d	a	d	a	d	a	d
17	1A92(A)	R13 / −74	I16 / −63	W20 / −173	G23 / −	L27 / −168	L30 / −75	L34 / −168	L37 / −173	I41 / −64	L44 / −123						
18	1GMJ(A)	I53 / −75	H56 / −74	I60 / −74	L63 / −65	I67 / −70	H70 / −73	I74 / −71	L77 / −67	E81 / −161							
19	1Q05(A)	K81 / −174	T84 / −54	V88 / 165	I91 / −62	I95 / −68	L98 / −61	R102 / −170	L105 / −69	A109 / −	C112 / 171						
20	1YF2(A)		I174 / −65	L178 / −65	I181 / −56	I185 / −66	I188 / −68	I192 / −71	L195 / −157	K199 / 168	L202 / −65	L206 / −93					
21	2C2A(A)	L285 / −56	L288 / −115	L292 / −112	I295 / −71	S299 / −76	L302 / −160	L306 / 179	L309 / 174								
22	2AYU(A)	V92 / 174	K95 / −55	L99 / −110	L102 / −107	L106 / −115	V109 / −166	F113 / 173	E116 / −69	L120 / −172	K123 / 172						
23	1ZHC(A)	F19 / 95; V46 / −168	I22 / −49; M49 / −61	H26 / 177; K53 / −154	L29 / −137; L56 / −94	I33 / 46; I60 / −75	A36 / −159; M63 / −162	N40 / −90; Y67 / −154	K70 / 73								
24	1K1F(A)	V28 / 168	I31 / −43	L35 / −169	A38 / −	I42 / −74	L45 / −64	V49 / 170	E52 / −63	M56 / −	L59 / −65	L63 / 64	E66 / −178				
25	1ENV(A)	W117 / −171	A30 / −	L34 / −136	I37 / −74	Q41 / −59	L44 / −108	I48 / −73	Q51 / −76	L55 / −87	T58 / 62						
	1ENV(A)		W120 / −177	I124 / −87	Y127 / −77	I131 / −58	L134 / −87	S138 / −64	Q141 / −103	N145 / −66	E148 / −77	L152 / −93					
26	1JAL(A)	L162 / 176	A133 / −	L137 / 178	C140 / 179	I144 / −79	L147 / −70	A151 / −	G154 / −								
	1JAL(A)		M165 / −64	L169 / 172	L172 / −63												
27	1QVR(A)	I403 / −80	L406 / −54	K410 / −179	L413 / −50	R417 / 70	L420 / −62										
	1QVR(A)		I435 / −179	I439 / −79	L442 / −82	I446 / −69	L449 / −62	W453 / −179	E456 / −89								
	1QVR(A)		I459 / −61	L463 / −161	A466 / −	L470 / 171	V473 / 167	I477 / −72	A480 / −	Y484 / 176	N487 / −49	E491 / 59					
	1QVR(A)		R493 / −174	L497 / 172	L500 / −49	V504 / 94	L507 / −59	L511 / −65									

Table 3. Angle χ_1 for residues in the **a**- and **d**-positions of trimers

No.	PDB ID	a	d	a	d	a	d	a	d
1	1AQ5(A)	Q18	V21	I25	L28	L32	V35	I39	L42
		–88	154	–148	–84	160	142	–80	–74
2	1B08(B)	V1204	L1207	V1211	L1214	V1218	L1221	F1225	Y1228
		–	–49	177	–75	175	–79	–158	–88
3	1EQ7(A)		S2	I6	L9	V13	L16	V20	L23
			65	–72	–74	167	–80	166	–107
		A41	A44	L48	M51	Y55			
		–	–	–78	60	–61			
4	1SWI(A)	M2	L5	V9	L12	A16	L19	V23	L26
		–49	–128	175	–78	–	–64	147	–98
5	2BEZ(C)	Y899	Q902	A906	F909	I913	I916	L920	T923
		–	–	–	178	–82	–77	–64	–64
			V934	A938	L941	V945	L948	F952	I955
			162	–	–173	174	–61	–75	–68
6	1G2C(A)		L160	V164	I167	L171	T174	V178	L181
			–174	172	–74	–146	–72	171	–175
7	1COS(B)	W2	L5	L9	L12	L16	L19	L23	L26
		–173	–56	–90	–82	–82	–154	–63	–34
	1COS(C)	–60	–83	–115	–65	–94	–80	–78	163

No.	PDB ID	a	d	a	d	a	d	a	d
1	1AQ5(A)	I46							
		–68							
2	1B08(B)	E1232							
		–133							
3	1EQ7(A)	V27	M30	V34	A37				
		170	–140	178	–				
4	1SWI(A)	V30							
		141							
5	2BEZ(C)								
		L959	I962	L966	V969				
		–67	–71	–115	156				
6	1G2C(A)	V185	L188	V192	L195	I199	Q202	I206	K209
		168	177	165	–74	–64	–62	67	–
7	1COS(B)								

Table 4. Angle χ_1 for residues in the **a**- and **d**-positions of tetramers-1

No.	PDB ID	a	d	a	d	a	d	a	d	a	d
1	2BNI(A)	M2	I5	L9	I12	G16	I19	L23	I26	L30	
		–59	–69	–77	–70	–	–69	–69	–77	–56	
2	2B1F(B)	V2	L5	V9	L12	N16	L19	V23	L26	V30	
		–69	–70	169	–71	–151	–178	165	–62	167	
3	1W5K(A)	M3	I6	L10	I13	L17	I20	L24	I27	L31	
		–170	–68	–73	–77	–82	–72	–70	–73	–68	
4	1C94(A)	R4	V7	L11	V14	L18	N21	L25	V28	L32	M35
		57	168	–88	162	–146	–77	–150	169	–91	49
5	4HB1(A)		L4	L8	A11	L15	A18	A22			
			175	–63	–	–66	–	–			
6	1GCL(A)	M2	I5	L9	I12	L16	I19	L23	I26	L30	
		–59	–87	–77	–58	–71	–82	–49	–67	–95	

Table 5. Angle χ_1 for residues in the **a**- and **d**-positions of tetramers-2

No.	PDB ID	a	d	a	d	a	d	a	d	a	d	a	d	a	d	a	d	a	d
1	1SFC(A)	L32 / 175	T35 / –53	V39 / 177	V42 / –173	M46 / –67	N49 / –79	V53 / 109	R56 / 169	L60 / –79	L63 / 178	A67 / –	L70 / –177	A74 / –	F77 / –179	A81 / –	L84 / –151	Y88 / –61	K91 / 170
	1SFC(B)		A191 / –	I195 / 177	R198 / –177	I202 / –67	L205 / 177	I209 / –80	L212 / –174	F216 / –84	M219 / –82	V223 / –22	Q226 / –47	I230 / –69	I233 / –64	V237 / 173	A240 / –		
	1SFC(C)		S25 / –75	T29 / 57	M32 / –76	V36 / –67	S39 / –46	G43 / –											
	1SFC(D)		T46 / –60	L50 / –134	Q53 / –73	L57 / –68	V60 / 163	M64 / –140	I67 / –64										
2	1GL2(A)	V12 / 175	L15 / –152	V19 / 169	V22 / 172	M26 / –63	N29 / –79	I33 / –	R36 / –165	L40 / –77	L43 / 178		L50 / 174	S54 / 70	F57 / –180	S61 / –67	V64 / 64		
	1GL2(B)	M168 / –	R171 / –173	I175 / –69	L178 / –175	I182 / –73	I185 / –70	F189 / –92	L192 / 173	I196 / –77	Q199 / –80		I206 / –72	V210 / 170	A213 / –	V217 / 169	A220 / –		
	1GL2(C)	I146 / –69	S149 / –73	A153 / –	T156 / –64	G160 / –	I163 / –75	L167 / –72	Q170 / –63	L174 / –70	T177 / –62	I181 / –70		L188 / –75	S191 / –60	L195 / –72		A199 / –	M202 / –57
	1GCL2(D)	L155 / –77	L158 / –179	I162 / –65	Q165 / –111	G169 / –	I172 / –70	L176 / –69	Q179 / –84	I183 / –69	L186 / –84			L197 / –109	E200 / –66				
3	1HVV(D)	I195 / –78	R198 / 177	I202 / –69	L205 / –180	I209 / –70	L212 / 177	F216 / –67	M219 / 179	V223 / 171	Q226 / –64	I230 / –69	I233 / –74	V237 / 168	A240 / –66	V244 / –56	A247 / –		
4	1VDF(A)*		M33 / –61	L37 / –62	T40 / –63	L44 / –93	V47 / 163	L51 / –101	Q54 / –169	L57 / –69	L61 / 174	V65 / –170	C68 / –177						
5	1NHL	A36 / –	S39 / 173	G43 / –	T46 / –57	L50 / –79	Q53 / –159	L57 / –69	I60 / –70	L64 / –100	I67 / –65								
6	1JTH(A)	D4 / –	M7 / –	L11 / –	M14 / –65	A18 / –	L21 / –72	S25 / –65	S28 / 176	M32 / –74	L35 / –73	S39 / –58	A42 / –						
	1JTH(A)			L57 / –66	I60 / –74	M64 / –67	I67 / –62	M71 / –84	I74 / –78	L78 / –62	L81 / –67								
	1JTH(B)	L50 / –69	Q53 / –71																
7	2B1F(D)	I195 / –61	R198 / –73	I202 / –73	L205 / –176	I209 / –78	L212 / –161												
8	4HB1(A)	L5 / –67	A8 / –	L12 / –	L15 / –66	L19 / –	A22 / –	L26 / –65											
9	1GCL(A)	M2 / –59	L5 / –87	L9 / –77	I12 / –	L16 / –71	I19 / –	L23 / –49	L30 / –95										
10	1G1I(A)		I95 / 48	M99 / –85	V102 / –58	M106 / –77	Q109 / –69	I113 / –65	L116 / –159	E120 / –66									
11	1HTM(B)**	N49 / –88	L52 / 174	I56 / –62	T59 / 66	F63 / –81	I66 / –63	F70 / –92	V73 / 147	I77 / –64	L80 / 180	V84 / 168	T87 / –75	L91 / –77	Y94 / 176				

Notes: * Pentamer.
** Trimer.

and other α-helical proteins (see [9, 10]), which are a subject of our further studies.

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