BEST EXPERIMENTAL PARAMETERS OF THE α-HELIX FROM PROTEIN CRYSTALLOGRAPHIC DATA

THE determination of the structures of globular proteins to the atomic detail using X-ray diffraction technique, has, in recent years, reached a good degree of accuracy with the crystallographic R-factor around 25% being quoted[1] and values around 12% for small proteins[2]. The coordinates are accurate to about 0·2 Å in many cases with a higher accuracy of about 0·1 Å being not ruled out for smaller proteins.

New methods and techniques for extracting the wealth of information from structural data have recently been proposed[3,4] and their utility demonstrated[5,6]. These have led to a better visualisation and characterisation of protein chain-folding. In fact, an indirect bonus was the observation of a new secondary structure of protein[7], to which the authors were led from the study of the θ chain plot.

TABLE I
Helical and statistical parameters for H, H_1 and H_3 helices

Helix	t (°)	h (Å)	r_N (Å)	r_C^α (Å)	r_C^1 (Å)	r_O (Å)	$\sigma(\eta)$ (°)	$\sigma(\eta_{ij})$ (°)
H	58.7 (20.7)	1.51 (0.37)	1.62 (0.40)	2.40 (0.62)	1.82 (0.43)	2.15 (0.41)	3.9	10.6
H_1	100.9 (2.4)	1.49 (0.05)	1.56 (0.15)	2.30 (0.14)	1.72 (0.09)	2.04 (0.14)	1.5	1.7
H_2	100.2 (2.2)	1.50 (0.06)	1.54 (0.10)	2.27 (0.10)	1.68 (0.11)	2.00 (0.10)	1.9	2.2
Best Value*	100.5 (2.3)	1.495 (0.055)	1.55 (0.13)	2.28 (0.12)	1.70 (0.10)	2.02 (0.12)		

* Mean of H_1, H_2 helices.

Besides these, the methods could be extended readily to the study of the helical regions in a protein. Details of these, which involve the use of η_{ij} plots, the stereogram and statistical parameters, devised for this purpose, are reported elsewhere[8]. The object of this note is to present one final result that could be arrived at from these applications, namely the calculation, from experimental data, of the "best" values (best in the least-squares sense) of the helical parameters for the α-helix, the data used being those of myoglobin (Perutz, personal communication to Professor R. Srinivasan). It turns out that the best helical regions are to be found in the H-helix. Judged from η_{ij} plot, the stereogram and the statistical parameters for details see ref. 8 this helix shows a clear bend with two sub-helical regions H_1 (residues 133 to 139) and H_2 (residues 142 to 149). The angle between these two subhelices is 11°[2].

With the use of radial and helical projections the least-squares fit for the best helical parameters have been deduced from the two sub-helices and are given in Table I. The values agree with the earlier values of Pauling[11]. As far as the authors are aware the values reported here are the first precise experimental determination from protein crystallographic data of the α-helical parameters.

We wish to thank Dr. M. F. Perutz for providing us with the latest coordinates of myoglobin.

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May 18, 1977.

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