

Fig. 2 Plot of the difference (Δ) between the two curves shown in Fig. 1.

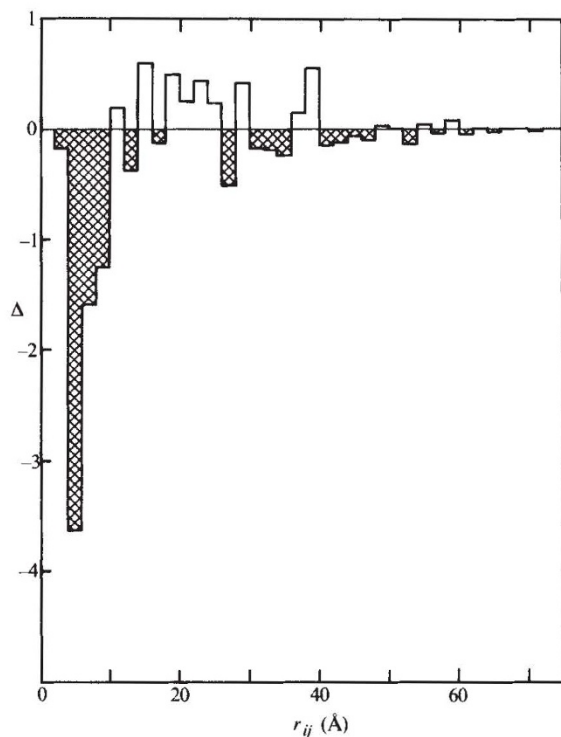


Fig. 3 Difference plot showing the distribution of separation between the dipolar charge and all ionic and dipolar charges (ion-pair interactions are ignored in this plot). 13,258 pairs from 14 proteins are included.

static energy which may tend to produce the Debye-Hückel-type charge distribution in proteins encounters two problems: the ambiguity of the value of the internal dielectric constant in protein and the estimation of the contact surface of the protein with water. Although the internal dielectric constant has been estimated⁷ to be in a range of 1–~60, here we adopted the value 4 as an averaged value because it is that most often used in

Table 1 The energy of charge-charge interaction in 14 proteins

	U_{ei} per protein (kcal mol ⁻¹)	U_{ei} per charged residue (kcal mol ⁻¹)	U_{ei} per α -helix end (kcal mol ⁻¹)
Myoglobin (deox.) (sperm whale)	-454	-13.7	-4.4
Concanavalin A (jack bean)	-168	-5.6	—
Lysozyme (hen egg-white)	-71	-3.6	-2.8
Papain (papaya latex)	-126	-3.7	-3.6
Ribonuclease A (bovine pancreas)	-75	-3.0	-7.1
Trypsin inhibitor (bovine pancreas)	-7	-0.3	-3.8
Adenylate kinase (porcine muscle)	-362	-8.8	-4.6
Carboxypeptidase A (bovine pancreas)	-338	-8.3	-1.4
Glyceraldehyde-3-phosphate dehydrogenase (lobster)	-563	-11.4	-2.4
Alcohol dehydrogenase (horse liver)	-595	-10.8	-2.3
Lactate dehydrogenase (dogfish muscle)	-452	-7.9	-4.4
Cytochrome C (ox.) (tuna heart)	-71	-2.6	-4.4
Carbonic anhydrase B (human)	-326	-8.3	-4.7
β -Trypsin (pH 8) (bovine pancreas)	5	0.6	-1.9

U_{ei} is the total electrostatic energy. U_{ei} is the energy of the interaction between ionic and dipolar charges. The internal dielectric constant of the protein, ϵ , is assumed to be 4.

similar calculations. The Tanford-Kirkwood algorithm contains the internal dielectric constant, so that, in principle, α_{ij} is affected by it. However, at neutral pH, the condition of the present calculation, the geometric parameter α_{ij} changes little with a change in the internal dielectric constant. A spherical contact-surface was simply assumed, and its radius was calculated from the molecular weight and the partial specific volume. The resulting electrostatic energies of the proteins are listed in Table 1.

The ionic charge is found to obtain an electrostatic stabilizing energy of several kcal per ionic residue, and the apparent charge of the α -helix dipole dose also has the same order of energy per helix end. Thus the present statistical examination shows that, on average, the electrostatic interaction among the ionic and the dipole constituents exceeds the energy of thermal agitation, and, therefore, that they are located so as to stabilize the protein structure.

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Erratum

THE words on the cover of *Nature* of 10 September 1981 (issue no. 5828) were incorrect and should have read 'Newly generated nuclei in adult rods'. The cover photograph (relating to the letter 'Genesis of rods in teleost fish retina' by P. R. Johns and R. D. Fernald *Nature* **293**, 141–142) was taken by R. D. Fernald and E. Newman of the Institute of Neuroscience, University of Oregon.