The structure of 2-keto-3-deoxy-6-phosphogluconate (KDPG) aldolase has been extended to 2.8 Å resolution using MIR methods. The final MIR phases were improved further with 3 cycles of refinement via electron density modification procedures coupled with fast Fourier transform phase angle calculations. With the complete sequence of the enzyme now available, a Kdrew model was constructed corresponding to the electron density of the final cycle. All 225 residues have been accounted for in the model. The main chain density is generally good except in the side chain density, while 21 residues are Gly.

The distribution of salt bridges and charged groups in proteins of known structure has been analysed. The survey includes residue type, conformation, accessibility, and specific interactions between termini, relationship to the active site and functional regions, domain linking and dimerisation and the asymmetry of the termini. The results suggest that the termini fulfill certain specific roles in maintaining the stable native conformation.

1. A survey of the N and C terminal regions in proteins of known structure has been performed. We have considered conformation, accessibility, proximity and specific interactions between termini, relationship to the active site and functional regions, domain linking and dimerisation and the asymmetry of the termini. The results suggest that the termini fulfill certain specific roles in maintaining the stable native conformation.

2. The similarity between the structure of 2-keto-3-deoxy-6-phosphogluconate aldolase and TIM was originally recognized by Richardson and Richardson's proposed reconnections are necessarily approximately correct as the a-helical periphery of the molecule probably affected the generally weaker interior density adversely at lower resolution.

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