

ATOMIC COORDINATES FOR TRIOSE PHOSPHATE ISOMERASE FROM CHICKEN MUSCLE

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Summary: Atomic coordinates are presented for the 3740 atoms other than hydrogen in the dimeric molecule of chicken muscle triose phosphate isomerase. They are derived from an electron-density map at 2.5Å resolution, interpreted in terms of the known amino-acid sequence, and they have been adjusted systematically to give stereochemically appropriate bond lengths and angles.

The three-dimensional structure of chicken muscle triose phosphate isomerase (D-glyceraldehyde 3-phosphoketo isomerase, E.C. 5.3.1.1) has been determined crystallographically at 2.5Å resolution by the method of multiple isomorphous replacement in association with chemical sequence analysis (1). The crystals were orthorhombic, space group $P2_12_12_1$, with unit-cell dimensions $a = 106.01$, $b = 74.76$, $c = 61.74$ Å and with one dimeric molecule of 53,000 daltons in the asymmetric unit. Five isomorphous derivatives were used for phase determination: the mean figure of merit was 0.73 and the r.m.s. error in the electron density map $\sigma = 0.20\text{eÅ}^{-3}$ (2).

Interpretation of electron-density map

The map, which was plotted on sections perpendicular to the c -axis, was interpreted in terms of the known amino-acid sequence (3) by the construction of a molecular model from Kendrew components in a Richards comparator (4). The independent densities corresponding to the two chemically identical subunits were considered separately instead of being combined and a complete molecular model was built and measured.

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The average electron density corresponding to the main polypeptide chains was $0.52\text{e}\text{\AA}^{-3}$ with average densities of 0.49, 0.49 and $0.56\text{e}\text{\AA}^{-3}$ for the $\text{C}\alpha$, NH and CO groups respectively. There were 15 breaks ($\rho < \sigma$) in the continuity of the density for the main chain in subunit I and 9 breaks for subunit II. However, only one short section of polypeptide chain, residues 168-176 in subunit I, could not be followed easily in the density though the ends of the chains, residues 1-2 and 246-8, were in weak density in both subunits. The residues having weak main-chain density ($\rho < 2\sigma$) are identified by the letter M after the residue number in the Table.

The electron density for the side chains varied in quality but more than half of the amino-acid residues could be identified within a small range of possibilities from the density alone. However 33 side chains in subunit I and 22 in subunit II were in densities too weak to give reliable indications of their conformations. These are identified by the letter W in the Table. In addition it should be noted that the electron density was often weak at the positions of $\text{C}\beta$ or $\text{C}\gamma$ atoms: 31 of the residues in the dimer had breaks in the electron density at these positions and in 14 further residues the density was weak. In contrast, 7 side chains in subunit I and 16 in subunit II were a poor fit to strong electron density: these residues are denoted by the letter S in the Table.

Measurement of atomic coordinates

Atomic coordinates were measured from the Kendrew model. A grid with lines at 1 cm ($\equiv 0.5\text{\AA}$) intervals in the \underline{a} - and \underline{b} - axial directions was suspended in the Richards comparator and the \underline{x} - and \underline{y} - coordinates were measured by superimposing each model component in turn on its image in the semi-silvered mirror and reading the position on the grid. The \underline{z} -coordinates were determined by measuring the perpendicular distance of each model atom from the mirror with a steel ruler and converting these measurements to distances from the chosen origin of the unit cell. Tests showed that the coordinates could be read to within 0.2\AA .

Atomic coordinates in triose phosphate isomerase. Atoms are represented by conventional abbreviations (6) and those in subunit I appear first. Symbols indicating the quality of the electron density are included after (some residue numbers (see text)).

continued

Table 1 continued

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Table 1 continued

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Table 1 continued

A 4x4 grid of 16 small images. Each image shows a different pattern of black and white dots arranged in a 4x4 grid. The patterns represent different binary representations of the number 10, such as 1010, 1001, 1011, etc.

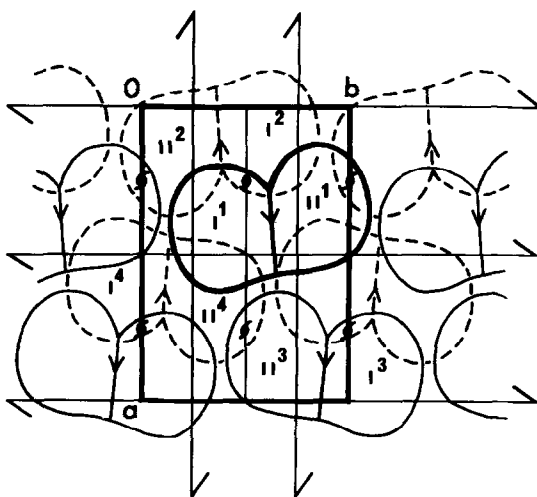
[illegible]

Adjustment to standard bond lengths and angles

The atomic coordinates were adjusted to give acceptable bond lengths and angles by the method of Dodson, Isaacs and Rollett (5). The r.m.s. shift in atomic position was 0.18\AA for subunit I and 0.11\AA for subunit II with maximum shifts of 1.34 and 0.60\AA respectively. The resultant bond lengths are distributed about standard values with standard deviations of 0.01\AA or less. Similarly bond angles have standard deviations of 2.6° . Peptide groups are closely planar with 175.2° the minimum ω -torsion angle (6).

Molecular symmetry

Analysis of the resultant atomic coordinates, which are listed in the Table, showed that the two subunits are well related by a non-crystallographic 2-fold axis of symmetry. The coordinates that are listed relate to a molecule centred at the point $\underline{x} = 40.36$, $\underline{y} = 46.25$, $\underline{z} = 0.32\text{\AA}$ and shown in heavy outline in the Figure. The axis relating C α atoms in the two sub-

Figure legend

Arrangement of molecules in the crystal structure. The coordinates listed relate to the molecule represented in heavy-outline. This and other molecules centred near $z/a = 0$ are shown in full line: molecules near $z/a = \pm \frac{1}{2}$ are shown in broken lines. The molecular axes are indicated by arrows within the molecular outlines. Subunits are marked I and II with superscripts 1-4 indicating the crystallographic equivalent positions (9).

units in this molecule (indicated by an arrow in the Figure) has direction cosines 0.9273, 0.0506, -0.3708 or, in spherical polar coordinates (7), its direction is defined by $\phi = 21.79^\circ$, $\psi = 87.10^\circ$. The subunits are related by a rotation defined by the Eulerian angles $\theta_1 = -86.57^\circ$, $\theta_2 = 136.47^\circ$, $\theta_3 = -92.82^\circ$ and a translation with components 7.33, 88.42 and 30.26 Å (8).

The r.m.s. separation of equivalent C α atoms in the two subunits when superimposed in this way is 1.20 Å. The corresponding figure for only those C α atoms involved in regular secondary structures is 0.78 Å.

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