ATOMIC CO-ORDINATES FOR DOGFISH M_4 APO-LACTATE DEHYDROGENASE

Margaret J. Adams*, Geoffrey C. Ford, Anders Liljas, Michael G. Rossmann

Department of Biological Sciences, Purdue University,
W. Lafayette, Indiana 47907 U.S.A.

Received April 3,1973

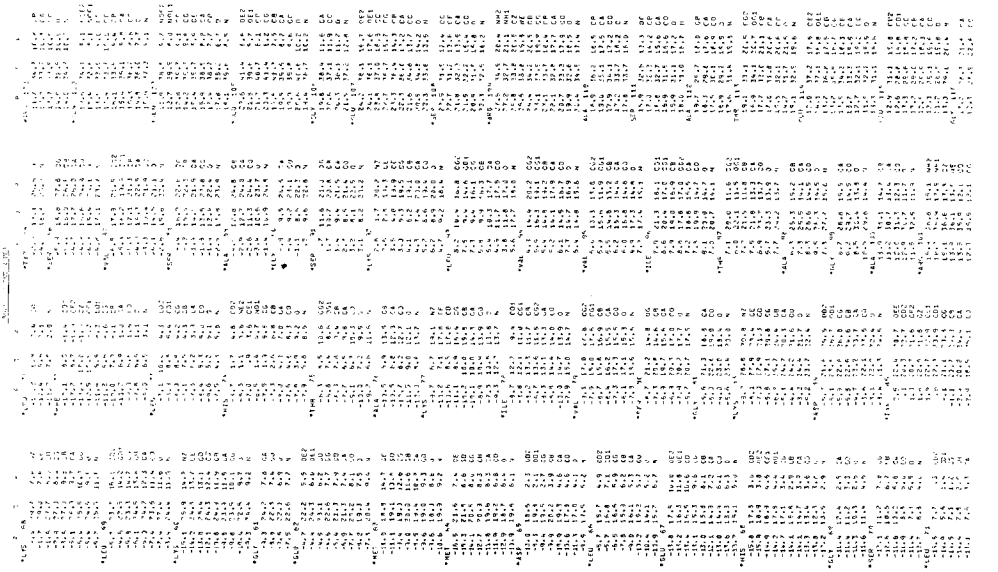
Summary: Atomic co-ordinates for one subunit of LDH are given in Å with respect to a Cartesian co-ordinate system corresponding to the molecular two-fold axes.

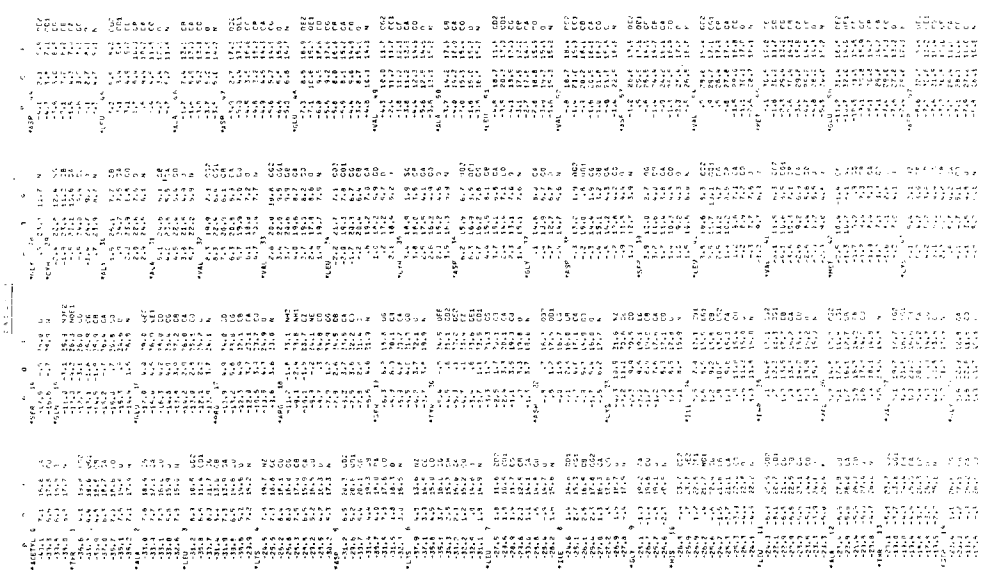
The structure of lactate dehydrogenase (LDH) has been described previously (1,2). The atomic co-ordinates of dogfish M_4 apo-LDH have now been measured on a model built with respect to a 2.0 Å resolution electron density map (3). One subunit was built with Kendrew skeletal models (Cambridge Repetition Engineers, Cambridge, England) in a Richards Optical Comparator (4). Co-ordinates were measured with two identical grids placed in position of suitably chosen electron density sheets. This reduced parallax in the measurement of those co-ordinates running parallel to the grids while giving an estimate of the co-ordinate which ran perpendicular to the grids.

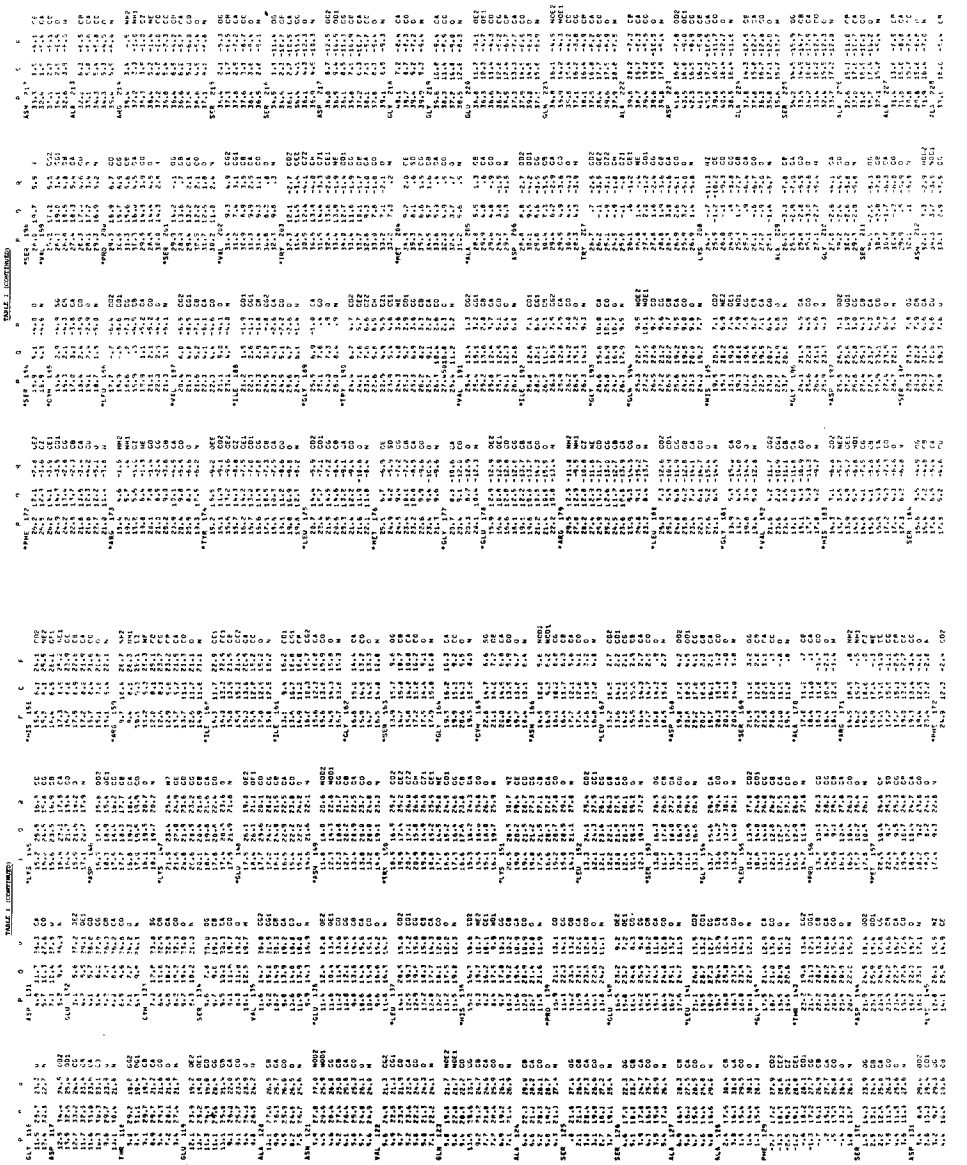
The co-ordinates were checked by a program which searched for unreasonable inter-atomic distances and angles. It also checked the hand of all asymmetric carbon atoms. These atomic positions were used as guide atoms in Diamond's model building program (5). Further refinement with respect to electron density is in progress using programs described by Diamond (6). Table I lists all atomic co-ordinates in Ångstroms with respect to the orthogonal molecular axes P, Q, R (7). Thus the standard ("red") subunit given in Table I is related to the "blue" subunit by a

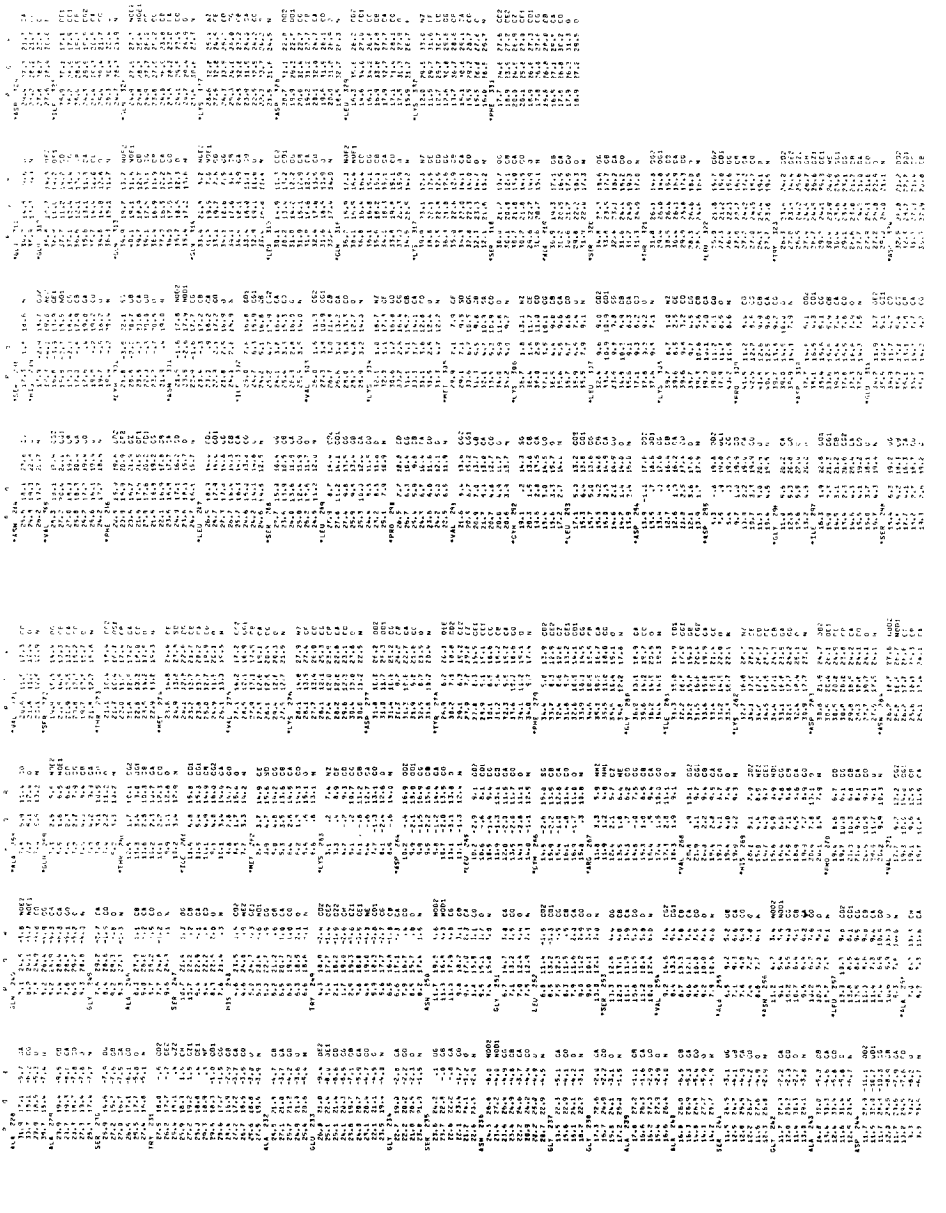
---

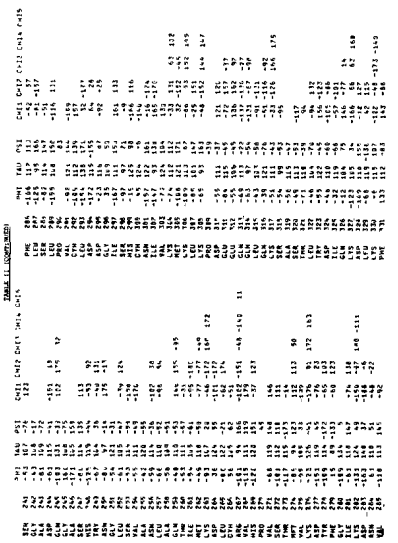
*Present address: Laboratory of Molecular Biophysics, Zoology Department, South Parks Road, Oxford, England.

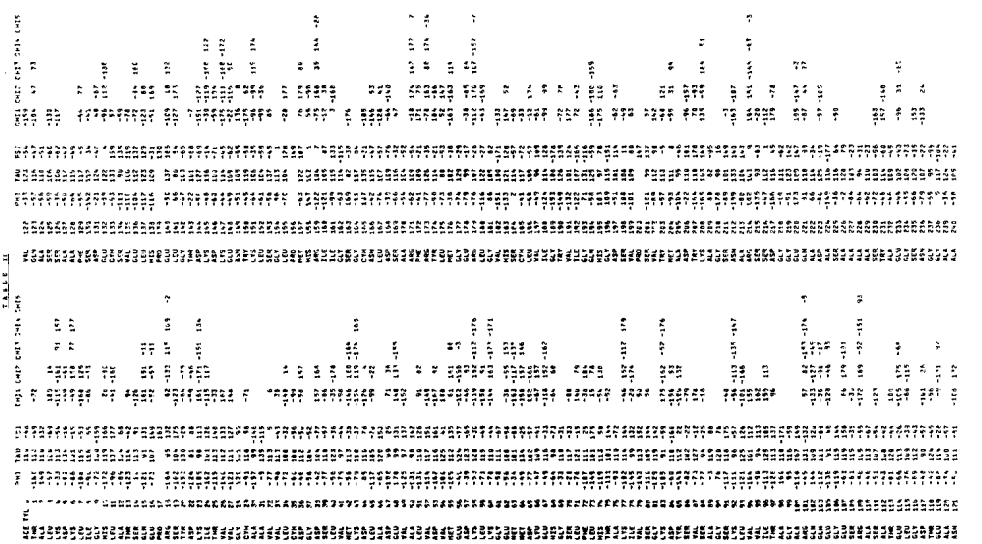












two-fold rotation about P, to the "yellow" subunit by a two-fold rotation about Q, and to the "green" subunit by rotation about R.

The amino acid sequence given in Table I, where marked by an asterisk, is in accordance with that of Taylor, Oxley, Allison, and Kaplan (8) in regions 1-109, 136-205, 253-331. The remaining portions have been given assignments based on the electron density map alone. The amino acid numbering system is that given by Rossmann et al. (2) which was based on the 2.5 Å resolution map alone. The deletions at positions 21, 82, and 104 and the insertion at 245 are based on improved electron density maps and recent chemical information (8). Apart from cysteine, which is referred to as CYH in Table I, the standard three letter code for amino acids is used.

Dihedral angles about main chain and side chain single bonds are given in Table II. The convention used for defining these angles is that suggested by the IUPAC-IUB Commission on Biochemical Nomenclature (9). The names allocated to the atoms in Table I similarily corresponds to those in the proposed IUPAC-IUB (9) nomenclature with transliteration of the Greek superscripts. The angle τ referred to in Table II is that contained by the main chain bonds NC^{α} and $C^{\alpha}O$.

REFERENCES

1. Adams, M. J., Ford, G. C., Koekoek, R., Lentz, P. J. Jr., McPherson, A. Jr., Rossmann, M. G., Smiley, I. E., Schevitz, R. W., Wonacott, A. J., Nature 227, 1098 (1970).
2. Rossmann, M. G., Adams, M. J., Buehner, M., Ford, G. C., Hackert, M. L., Lentz, P. J. Jr., McPherson, A. Jr., Schevitz, R. W., Smiley, I. E., Cold Spring Harbor Symp. Quant. Biol. 36, 179 (1971).
3. Adams, M. J., Ford, G. C., Lentz, P. J. Jr., Liljas, A., Rossmann, M. G., Proc. Nat. Acad. Sci., submitted for publication (1973), as an appendix to (8).
4. Richards, F. M., J. Mol. Biol. 37, 225 (1968).
5. Diamond, R., Acta Cryst. 21, 253 (1966).
6. Diamond, R., Acta Cryst. A27, 436 (1971).
7. Rossmann, M. G., Adams, M. J., Buehner, M., Ford, G. C., Hackert, M. L., Liljas, A., Rao, S. T., Banaszak, L. J., Hill, E., Tsernoglou, D., Webb, L., J. Mol. Biol., in press (1973).
8. Taylor, S. S., Oxley, S. S., Allison, W. S., Kaplan, N. O., Proc. Nat. Acad. Sci., submitted for publication (1973).
9. IUPAC-IUB Commission, J. Biol. Chem. 245, 6489 (1970).