The recombinant monomeric N-terminal heme-binding domain of the blood protein of the parasitic nematode Ascaris lumbricoides has an exceptionally high affinity for oxygen. It is an octameric protein containing two similar heme-binding domains per subunit. The recombinant monomeric N-terminal heme-binding domain (D1) retains full oxygen avidity. Its structure reveals a characteristic globin fold. A strong hydrogen bond between tyrosine B10 and the ligand distal oxygen, combined with a weak hydrogen bond involving the oxygen of the heme hydroxyl to dioxygen. Mutation of E7 Tyr side chain is still maintained. There appears to be no movement of the heme group, in contrast to the E7 Asn side chain of an Asp in this loop now appears to form a hydrogen bond, but a hydrogen bond to the B10 Tyr side chain is still maintained. There appears to be no movement of the heme group, in contrast to the E7 Q→L mutant, but the FG loop has moved further toward the exposed edge of the heme group.

Rotation and translation function procedures only reach correct results when powerful mathematical techniques are used to measure the goodness of fit between observed and calculated Patterson maps. Usually, Image Seeking Functions (ISF) [1] solve satisfactorily this problem. Several tests [2-3] based on computer generated random numbers showed how the behavior of the ISF depends largely on certain relations between statistical descriptors (such as mean and standard deviation) of the Patterson maps. Real data tests, now performed, confirm the previous results from computer simulation. Useful transformations of observed and calculated data will be suggested to improve the results when applying ISF.

PS02.07.15 MOLECULAR FEATURES OF OXYGEN AVIDITY DISCERNED FROM STRUCTURES OF ASCARIS HEMOGLOBIN DOMAIN I AND SEVERAL MUTANTS. F. Scott Mathews, Louise M. Curran, Jian Yang, Andrew P. Kloek and Daniel E. Goldberg. a,Department of Biochemistry and Biophysics, b,Department of Molecular Microbiology and Mathewsa, Louise M. Curanea, Jian Daniel E. Goldbergb,c. a,Department of Biochemistry and The recombinant monomeric N-terminal heme-binding domain of the blood protein of the parasitic nematode Ascaris lumbricoides has an exceptionally high affinity for oxygen. It is an octameric protein containing two similar heme-binding domains per subunit. The recombinant monomeric N-terminal heme-binding domain (D1) retains full oxygen avidity. Its structure reveals a characteristic globin fold. A strong hydrogen bond between tyrosine B10 and the ligand distal oxygen, combined with a weak hydrogen bond involving the oxygen of the heme hydroxyl to dioxygen. Mutation of E7 Tyr side chain is still maintained. There appears to be no movement of the heme group, in contrast to the E7 Asn side chain of an Asp in this loop now appears to form a hydrogen bond, but a hydrogen bond to the B10 Tyr side chain is still maintained. There appears to be no movement of the heme group, in contrast to the E7 Q→L mutant, but the FG loop has moved further toward the exposed edge of the heme group. 

PS02.07.16 HOW THE ATOMIC STRUCTURE OF A CRYSTAL CAN BE SEEN WITHOUT A HIGH RESOLUTION MICROSCOPE. V. L. Indenbom.

PS02.09.01 DIRDIF-96: PATTERSON METHODS, DIRECT METHODS ON DIFFERENCE STRUCTURES, AND COMPLEMENTATION OF THE STRUCTURE BY AUTOMATIC RECYCLING. Paul T. Beurskens, Randy Israel, Gezina Beurskens, Rene' de Gelder, W.P. Bosman and J.M.M. Smits, Crystallography Laboratory, University of Nijmegen, The Netherlands

Direct methods become more and more powerful every year, but some structures cannot be solved easily, because of poor data sets, low resolution data?, pseudo-symmetry?, heavy atoms?, or just bad luck?

The heavy-atom interpretation techniques in DIRDIF are fully automated and possible symmetry problems are solved by the special application of direct methods to difference structure factors. Vector search methods offer an ideal possibility to use your chemical knowledge. The expected geometry of a molecular fragment may be obtained from structural publications (your own research, the Cambridge Data Base) or by Molecular Modelling.

The intramolecular vectors are rotated in Patterson space, and acceptable orientations are positioned, all without user intervention: the programs are more powerful than the unexperienced user!

Finally, the heavy-atom structure, or the resulting structural fragment from the vector search techniques, is expanded to the full structure: again fast and fully automatic, using improved R3 recycling criteria, and new strategies for rejecting Fourier peaks by checking expected peak heights and molecular geometries. In most cases the structure is solved.

But if the heavy atoms are not so heavy, or if the Patterson allows homometric solutions, or if the molecular fragment is not unique or not completely correct or very small, a large number of tentative structural models may be obtained. User controlled recycling is then possible, but automatic multisolution-recycling is on its way: the program selects the most probable model (using various FOM's), tries to expand it to the complete structure, and if unsuccessful, selects the next probable model.

PS02.09.02 IMPROVEMENTS ON THE USE OF IMAGE SEEKING FUNCTIONS. Javier Borge, Santiago Garcia-Granda, Departamento de Quimica Fisica y Analitica, Facultad de Quimica, Universidad de Oviedo, C/ Julián Clavería, 8, 33006 Oviedo, Spain

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