

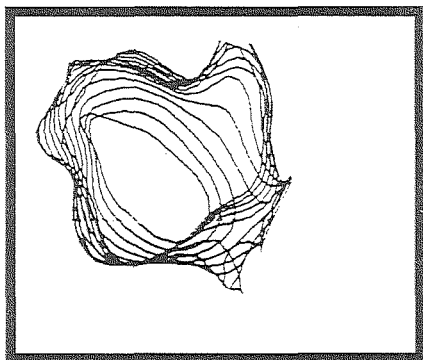
& Weber, *Nature*, 1988, 366, 403-405). The subunit of PCD from *P. aeruginosa* contains 438 residues, and that of *P. cepacia* 431. Both contain one nonheme iron atom. The identity between the two proteins is 48 percent, and there are many deletions and insertions. A conservative search model was used, consisting of 382 residues (1868 atoms) of a polyalanine (glycine) chain, from *P. aeruginosa*, with many gaps, and representing 1.6 percent of the unit cell contents of the *P. cepacia* PCD.

P. cepacia PCD crystallizes in $P2_12_12_1$ with four tetramers per cell. Ludwig *et al.* observed absences of odd orders of l in the hOl diffraction pattern, indicating the presence of a non-crystallographic local 2-fold axis at $x \approx 0.25$, and approximately parallel to c and suggesting that the local tetramer symmetry is 222. With a tetramer as the asymmetric unit, the rotational search with one monomer would normally give four symmetrically independent solutions. If a noncrystallographic 2-fold axis of the tetramer is parallel to a 2-fold axis in the Patterson, the rotation search solutions reduce to two correspondingly enhanced maxima. Thus the rotation search is facilitated by the orientation of the tetramer 2-fold axis. There is no corresponding enhancement of the maxima in the translation search.

With data to 2.9 Å resolution, the two maxima in the rotation search, mapped as the correlation coefficient, were 0.0809 and 0.0744, or 9.9 and 9.1 σ , respectively, in terms of standard deviations above the background. Spurious peaks were found at up to 3 σ ; among these were peaks resulting from an approximate 2-fold symmetry within part of the subunit (Ohlendorf *et al.*). The four symmetrically independent solutions to the translation search were found at 3.2 to 4.1 σ ; the known location of the non-crystallographic 2-fold axis made a fully exhaustive translation search unnecessary.

PS02.06.18 VERY LOW RESOLUTION PHASING ATTEMPTS OF THE RIBOSOMAL 50S PARTICLE FROM THERMOPHILUS BY THE FEW ATOMS MODEL METHOD. A.D. Podjarny, A.G. Urzhumtsev and E.A. Vemoslova, UPR de Biologie Structurale, IGBMC, B.P. 163, 67404 Illkirch Cedex, C.U de Strasbourg, France

A suggestion for the phases for the 80 Å resolution X-ray diffraction data from the 50S ribosomal particle of *Thermus thermophilus* (Volkman *et al.*, *J. Mol. Biol.*, 216, 239, 1990) has been made using the Few Atoms Model ab initio technique (Lunin *et al.*, *Acta Cryst.*, D51, 896, 1995), in collaboration with A. Yonath and coworkers. This technique generated randomly one million models consisting of 5 pseudo atoms each and selected the 560 solutions which fitted best the observed amplitudes to 60 Å resolution. The selected models were grouped with a clusterisation procedure in a small number of possible solutions. The most adequate one was chosen by imposing the additional constraint that



there should be no strong densities on symmetry axes. To refine this result, a second model generation was done imposing stronger amplitude constraints between 120 and 60 Å and density constraints based on the result of the first generation. The map resulting from the second model generation (phased to 80 Å) is shown in the figure. The position and features of the observed envelope agree with those obtained with other ab-initio solution methods and with molecular replacement using models from electron microscopy reconstructions (Volkman *et al.*, CCP4 Newsletter, 31, 23, 1995).

PS02.06.19 MOLECULAR REPLACEMENT METHOD USING A PARALLEL PROCESSING MACHINE. V.S. Yadava and K.K. Kannan Solid State Physics Division, Bhabha Atomic Research Centre, Bombay-400 085, INDIA.

The molecular replacement method involves six parameters - three rotational and three translational and the correct orientation and position is identified by calculating R-factor at each grid point.

Time requirement: The six-dimensional search requires very large amount of computer time. For a moderate size protein like Carbonic Anhydrase with about 2000 atoms in the molecule and 2000 reflections to 5Å requires 20 minutes of cpu time on a Landmark 860 machine for structure amplitude calculations at 1.5Å resolution along the axes for each orientation. For a coarse search with steps of 5 degree in Eulerian angles there are 46656 orientations which require 648 days of computer time. However, with a 64-node parallel-processing system the time required is 10 days of the machine time and can be further reduced by using more nodes and faster machines. Program implementation: As the calculations for each orientation are independent of that for others, the different orientations are equally distributed between different nodes. Each node has all the information for calculating structure amplitudes and Rvalue.

Results: The method has been tested first with Human Carbonic Anhydrase (HCA) I data and the same protein as model structure. Next HCA II was used as the model structure for obtaining structure of HCA I. Lowest R-value corresponded to correct orientation and position in both the cases.

PS02.06.20 AUTOINDEXING OF MULTIPHASE POLYCRYSTALS. V.B. Zlokazov FLNP JINR, 141980 Dubna, Moscow region, Russia. E-mail: Zlokazov@main1.jinr.dubna.su

Let a set of interplanar spacings (d_j), $j = 1, 2, \dots, m$ be given, which are diffraction reflections from a n -phase polycrystal. The autoindexing problem is solved by minimizing the following functional

$$\sum_{i=1}^n \rho(\vec{d}, \vec{f}(\vec{P}_i, \vec{h}_i)) + \alpha V(\vec{P}_i) + \beta N(\vec{P}_i, \vec{h}_i, \delta) \quad (1)$$

The first member is

$$\rho = \sum_{j=1}^m \delta_1 [d_j, f(\vec{P}_i, \vec{h}_j^*)] \quad (2)$$

where \vec{h}_j^* = index values, minimizing expressions

$$R_j = \delta_2 [d_j, f(\vec{P}_i, \vec{h}_j)] \quad (3)$$