01.4-12   REFINEMENT OF THE MONOCLINIC HEN EGG WHITE
            LYSOZYME AT 2A RESOLUTION. By S. T. Rao,
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Monoclinic crystals of hen egg white lysozyme grown at
pH 4.4 contain two independent molecules in the asymm-
etric unit with cell dimensions $\underline{a}$ = 28.0, $\underline{b}$ = 62.9,
$\underline{c}$ = 60.5A; β = 90.8°; space group $P2_1$. The backbone
chain was traced from a 4A MIR map phased with four
derivatives (Acta Cryst. B37 (1981) in press). The
tetragonal model fitted to this chain trace provided
the starting model for the two molecules. The phases
were extended to 2.5A using Mayer's graphics system
at Texas A&M and a model was rebuilt into a density
calculated with 2Fo-Fc as coefficients. Segments of
the polypeptide chain being fitted were excluded from
the phasing calculations. The model, comprising of two
molecules, was subjected to 20 cycles of difference
Fourier refinement followed by idealisation of stereo-
chemistry (Dodson, Isaacs & Rollett, Acta Cryst. A32,
311 (1976)). This model had a few short contacts
between side chain atoms in both the molecules. These
contacts have been relieved and the model coordinates
have been subsequently improved by two complete rounds
of 2Fo-Fc maps using the Vector-General graphics in
our laboratory, R = 0.29 for 6535 reflections. We
are now carrying out reciprocal space refinement at
2A (13,000 reflections) using the Konnert-Hendrickson
procedure.

01.6-01   CONTRAST VARIATION STUDIES IN LOW RESOLU-
TION NEUTRON CRYSTALLOGRAPHY : AN APPLICATION TO THE
NUCLEOSOME CORE PARTICLE. G.A. Bentley[x], J.T. Finch[+],
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The method of H_2O/D_2O contrast variation, which has
been successful in small angle neutron scattering to
distinguish protein and nucleic acid in complex macro-
molecules (e.g. chromatin, viruses), is being applied
to crystal structure determination at low resolution.
The neutron scattering cross-sections of H_2O and D_2O
are quite different and this property is used to match
the scattering density of either the protein or the
nucleic acid moieties in order to visualise each
separately.

The effect of solvent contrast on the low resolution
structure factors (d-spacing $\gtrsim$ 15 Å) may be usefully
exploited to obtain relative phase information inde-
pendent of any prior structural interpretation. For
centrosymmetric terms, the structure factor is a linear
function of the H_2O/D_2O ratio. This property may be
used to scale together data sets from crystals soaked
in different H_2O/D_2O buffers and to obtain the relative
phase change from one contrast to the next. In the case
of non-centrosymmetric structure factors the magnitude
of the relative phase change may be determined but not
its sign. These relationships, which depend only on the
magnitudes of the observed structure factors measured
in known contrasts, can be used to transfer phase in-
formation between the different H_2O/D_2O contrasts.

We have measured low-resolution 3-D data from crystals
of the nucleosome core particle at contrasts of 0 %
D_2O, 39 % D_2O (protein matched out) and 65 % D_2O (DNA
matched out). We shall describe the use of the contrast
variation method in solving the structure and its

ability to distinguish protein and DNA in low-resolution
crystal structure analysis.

The results show that the nucleosome core particle
consists of a central protein core surrounded by appro-
ximately 1.8 superhelical turns of DNA .

01.6-02   A SINGLE-CRYSTAL NEUTRON DIFFRACTION STUDY
OF SPERM-WHALE OXYMYOGLOBIN.   By S.E.V. Phillips, MRC
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Neutron diffraction data have been collected to approxi-
mately 1.7 Å resolution on large crystals of oxymyoglo-
bin in D_2O buffer, using the protein crystallography
station at the High Flux Beam Reactor, Brookhaven Nat-
ional Laboratory. The diffractometer was equipped with
a 2-dimensional multiwire detector, and a cooling device
to maintain a temperature of -5°C at the crystal to re-
tard oxidation of the haem iron. Two crystals were
used to collect 14,411 independent reflexions, the merg-
ing R between crystals being 14.1% on intensities.

An F_o-F_c map, phased from the refined X-ray co-ordinates
of C,N,O,S,Fe atoms, showed peaks for half the H and D
atoms. Adding all observed H and D atoms, and those
whose positions were known from stereochemistry, to the
model gave R=33% for 10,151 reflexions with I>1.5σ(I).
After 10 cycles of Jack-Levitt refinement (R=18.8%) a
difference map showed a strong peak for D bonded to N_ε of
His E7, indicating a good H-bond from the proximal
imidazole to the dioxygen ligand. The function of this
histidine in myoglobin and haemoglobin is to stabilize
the haem-oxygen complex.

The pattern of H/D exchange is clear in the maps, and
will be discussed, together with a description of hydro-
gen bonding and water structure.