01.5–2 REFINEMENT OF THE $C222_1$ CRYSTALLINE FORM OF OXIDIZED UTEROGLOBIN AT HIGH RESOLUTION. By I. Morize, E. Surcouf, M.C. Vaney, Y. Epelboin & J.P. Mornon, Laboratoire de Minéralogie-Cristallographie, CNRS LA 09, Université Paris 6, T 16, 4 place Jussieu, 75230 Paris Cedex 05, France.

The $C222_1$ crystalline form of Uteroglobin has been refined at 1.5 Å resolution starting from the isomorphous replacement model (J.P. Mornon, F. Fridlansky, R. Bally & E. Milgron, 1980, J. Mol. Biol., 137, 415-429), partially refined by energy minimization at 2.2 Å resolution by M. Buehner (Wurzburg University, FRG, private communication). Refinement has been performed using the Hendridkson-Konnert program (W.A. Hendrickson & J.H. Konnert, 1980, Biomolecular structure, function, conformation and Evolution, Vol 1, R. Srinivasan ed., 43-57) modified by W. Furey (W. Furey, B.C. Wang & M. Sax, 1982, J. Appl. Cryst., 15, 160-166). It has been adapted to our local facilities (CII-HB Mini 6/53 16 bits machine + AP 100 FPS array processor). Four ier calculations, vizualisation and manipulation have been performed by means of local softwares (DENSON, E. Surcouf & J.P. Mornon, 1983, local report) for graphic display and plotter, MANOSK (E. Surcouf & M.C. Vaney, 1984, local report) for PS 300 Evans & Sutherland interactive color display). At the present stage, 66 cycles give a crystallographic R close to 0.22 for 12400 reflexions ($|F|>\sigma|F|$). Most of the residues are accurately localized. Water molecules have been included in the model. The study of the central cavity, previously detected in Uteroglobin, is of special interest. This hydrophobic cavity is probably well suited to bind a steroid, likely Progesterone (E. Surcouf, 1982, Thesis). In the refined $C222_1$ molecule the cavity appears to be occupied only by disordered water molecules trapped inside the protein. So, on the 6th day of gestation, when Uteroglobin was extracted from rabbit Uteri (F. Fridlansky & E. Milgron, 1976, Endocrinology, 99, 1244-1251) it does not probably carry a steroid. It seems also, from the present result and from our previous observations (unpublished data), that the other crystalline forms of oxidized Uteroglobin are built with substrate free protein molecules.

01.5–3
ANISOTROPIC X-RAY REFINEMENT OF RIGID GROUP VIBRATIONS IN PROTEIN STRUCTURES
By D.S. Moss and I. Haneef, Department of Crystallography, Birkbeck College, Malet Street, London WC1E 7HX, UK.

The data-to-parameter ratio in protein structure refinements is usually not sufficiently favourable to allow free anisotropic refinement of thermal parameters. By making reasonable assumptions about the atomic motions, the number of parameters may be reduced.

Some groups of atoms in protein structures exhibit dynamic or static disorder which may be approximated by rigid body displacements. Notable among such groups are the planar rings of phenylalanine, tyrosine, histidine and tryptophan residues where non-rigid body vibrations have mean-square amplitudes ($<0.01Å^2$) much smaller than observed in protein crystal structures ($>0.1Å^2$).

We have applied the TLX approximation to the refinement of several rings in ribonuclease at 1.45Å resolution, including the catalytically important His-119 where relative site occupancy has also been refined to allow for anhamonic nature of the disorder.

The results have been analysed in terms of librations about side-chain chemical bonds.

01.5–4 THE REFINEMENT OF SOUTHERN BEAN MOSAIC VIRUS IN RECIPROCAL SPACE. By Abelardo M. Silva[+] and Michael G. Rossmann, Department of Biological Sciences, Purdue University, West Lafayette, Indiana 47907, USA. [+]Present Address: Departamento de Fisica, Facultad de Ciencias Exactas, U. N. de La Plata, C. C. No. 67, 1900 La Plata, Argentina.

The restrained least-squares procedure of Hendrickson-Konnert (Konnert, J. H. & Hendrickson, W. A., Acta Crystallogr. A36, 344-350, 1980) has been applied to native southern bean mosaic virus diffraction data extending to 2.88 Å resolution. The initial model, based on a multiple isomorphous replacement map improved by three cycles of real-space molecular replacement averaging, gave an overall R-factor of 40.7%. Subsequent to refinement after 65 cycles and numerous model checks in a computer graphics system, using the Jones FRODO program (Jones, T. A., J. Appl. Crystallogr. 11, 268-272, 1978), the R-factor decreased to 25.5%. The refinement required vectorization of the program on the Cyber 205 computer and the selection of partial data sets, compensated by the presence of non-crystallographic symmetry. Furthermore, non-crystallographic symmetry was used as a constraint rather than restraint, thus reducing the number of independent variables by a factor of 10. About 40 water molecules per icosahedral asymmetric unit were identified. A small region in the interior of the virus but bordering on the inner protein surface is probably a small portion of RNA with partial icosahedral symmetry.

01.5–5 THE ANISOTROPIC REFINEMENT OF 2-Zn PIG INSULIN STRUCTURE AT 1.2Å RESOLUTION. By W. R. Chang, D. Stuart, J. B. Dai, R. Todd, J. P. Zhang, D. L. Xie, B. Kuang and D. C. Liang, Institute of Biophysics, Academic Sinica, Beijing, China.

A set of data at 1.2Å resolution collected with 34 crystals at 7-10°C was corrected for radiation damage, absorption, scaling factor and temperature factors. The reciprocal space refinement was restrained by the incorporation of extensive chemical observations into least-squares equations programmed by W. Hendrickson. Two cycles of refinement were carried out for all the non-hydrogen atoms of the insulin dimer with anisotropic temperature factors after the isotropic refinement for non-hydrogen and hydrogen atoms of the protein with water molecules and bulk solvent. The agreement factor (R) dropped to 13% and the rms deviation from ideal covalent bond lengths was 0.02Å. The electron density of most hydrogen atoms was found on the D-maps calculated without the contribution of hydrogen atoms. Anisotropic distribution of electron density of sulphur atoms and some other non-hydrogen atoms can be seen clearly on the map and the fit with the density was improved distinctly after anisotropic refinement. The water structure and the anisotropic vibration of atoms will be discussed.