02.8–2 X-RAY DIFFRACTION PATTERNS FROM SINGLE CRYSTALS OF LARGE RIBOSOMAL PARTICLES FROM B. STEAROTHERMOPHILUS. By A. Yonath*,H.D.BARTUNIK**; K.S.BARTELS**,H.-G.WITTMANN+; * Weizmann Institute Rehovot, Israel; ** EMBL, c/o DESY,Hamburg,FRG; + Max-Planck-Institut f. Molekulare Genetik, Berlin, FRG.

The full understanding of the process of protein biosynthesis still awaits a structural model.To this end we have attemped crystallographic studies on ribosomes.

Three dimensional crystals of intact 50S ribosomal particles from B.stearothermophilus have been obtained by us.These crystals grow in vitro, within several weeks, by a modified version of the vapour diffusion technique.They grow reproducibly,reach dimensions of 1x0.2x0.1mm and are rather fragile.Preliminary X-ray diffraction patterns of native and cross-linked single crystals have been obtained,mainly with synchrotron radiation (DORIS/X11 at EMBL/DESY). These extend to 10-15Å resolution and indicate packing in relatively small unit-cells, reasonable degree of internal order and adequate stability in the X-ray beam.

X-ray diffraction data from samples containing large number of micro crystals show sharp rings, among them some with spacings that agree well with those of gels and of solutions of ribosomes. The low resolution "powder" diffraction patterns indicate packing that accords with that of the single crystals.

02.8–3 THE STRUCTURE OF RIBOSOMAL PROTEINS FROM A THERMOPHILIC BACTERIUM. by K.Appelt, S.W.White, and K.S.Wilson* of Max-Planck Institute for Molecular Genetics, Abt.Wittmann, Ihnestrasse 63-73, 1000 Berlin 33.

We have been studying the crystal structures of ribosomal proteins from the thermophilic eubacterium Bacillus stearothermophilus. The proteins are extracted from the ribosome by mild methods with 1 or 2 molar salt solutions to avoid denaturation of the native structures during preparation.

We have crystals of three of the 52 proteins: L30 and L6 from the large sub-unit and S5 from the small sub-unit. S5 in fact occupies a position close to the interface between the 30S and 50S ribosomal sub-units. The numbers given are based on established sequence homology to the E.coli proteins: proteins from the organisms have identical residues at about 50% of the positions with almost no deletions/insertions being required for optimum alignment.

We have interpreted the structure of L30 at 2.5Å resolution. The structure is composed of a 3-stranded beta sheet and two helical segments. The molecule is extremely compact and globular. We have analysed S5 and L6 at low, 6Å, resolution, and will extend the resolution in the near future. The low resolution maps again indicate compact conformations for the proteins.

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02.8–4 **A MOLECULAR MODEL FOR CODON-ANTICODON$_{Asp}$ RECOGNITION : THE CRYSTAL STRUCTURE OF YEAST tRNA^{Asp}.** **By D. Moras, P. Dumas, R. Giegé and E. Westhof, Institut de Biologie Moléculaire et Cellulaire du CNRS, 15, rue Descartes 67084 Strasbourg - France**

One of the interesting characteristics of the nucleotide sequence of yeast tRNA^{Asp} is the self-complementarity of the anticodon triplet GUC. This feature induces the formation of tRNA dimers in solution and in the crystalline state as shown by the crystal structure of yeast tRNA^{Asp} in its orthorhombic form.

The structure of yeast tRNA^{Asp} has now been refined to 3Å resolution using the restrained least-squares method of Hendrickson and Konnert and the graphic modelling programm FRODO of A. Jones. The conventional R-factor is 23% for 4585 significant reflexions ($F > 2\sigma F$).

In the anticodon loop, G34 and C36 form two Watson-Crick base pairs with C36 and G34 of a twofold symmetrically related molecule. A water bridge relates the two central uridines. The stacking of the modified base G37 on both sides of the triplet stabilizes the interactions. The resulting helical stack is in the continuity of the anticodon stem.

Anticodon-anticodon association rigidifies the related loops, as shown by the distribution of the temperature factors when compared with the corresponding values in the structure of yeast tRNA^{Phe}. The interaction results in a conformational charge which propagates along the anticodon double helical stem. This is a clear example of the flexibility of nucleic acids.

02.9–1 STRUCTURE OF $_1$A GRAMICIDIN A/CESIUM$_2$COMPLEX. B.A. Wallace[1] and W.A. Hendrickson[2], [1]Department of Biochemistry, Columbia University, New York, N.Y. 10032 and [2]Laboratory for Structure of Matter, Naval Research Laboratory 6030, Washington, D.C. 20375 U.S.A.

Gramicidin A, a linear polypeptide antibiotic, forms channels in phospholipid membranes which are specific for monovalent cations. Dimers of this hydrophobic molecule adopt very different conformations in membranes and in organic solvents, and different crystal forms have been prepared in the presence and absence of ions and/or lipid molecules [Wallace, Biopolymers 22, 397 (1983)]. Crystals of one gramicidin/ion complex which diffract to 1.5 Å have been prepared from a CsCl solution in methanol (Kimball and Wallace, Ann. N.Y. Acad., in press). This crystal form (space group $P2_12_12_1$, a=32.11, b=52.10, c=37.16 Å) contains 2 dimers per asymmetric unit. Because of the high cesium content in these crystals, the Bijvoet differences from the cesium ions are calculated to be ~16% with a Cs^+ partial structure contribution of 71% in F, so it was possible to calculate a 1.8 Å electron density map using single wavelength anomalous scattering for phasing. This preliminary map reveals the helical structure of the molecule and the cation-binding sites. Attempts to fit the polypeptide chain are now underway.

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