The crystal structure of SN6999 bound to the DNA sequence d[CGC(O^6-ethyl-G)AATTCGCG] is presented. The space group is $P2_12_12_1$ and the unit cell dimensions are a=28.48Å, b=36.11Å, c=69.6Å. A new lattice packing is observed and the structure was solved by molecular replacement using ULTIMA. A canonical d[CGCGAATTCGCG] dodecamer crystal structure was used as the search model. The asymmetric unit contains one dodecamer duplex, one SN6999 and 67 water molecules. The structure was refined against 1618 2σ(F) reflections extending to 2.25Å resolution by constrained least squares using NUCLSQ to an R-factor of 17.0%. SN6999 distorts the double helix at the C1 to e^6G4 end. The new lattice retains the interlocking interactions between the terminal CG base pairs in the minor groove. The e^6G4:C21 base pair is distorted while e^6G16:C9 shows a bifurcated base pair. Supported by NIH grants GM-41612 and CA-52506 to A.H.-J.W.

PS-04.02.10 CRYSTAL AND MOLECULAR STRUCTURE OF A HEXADECAHYDRATED 2:1 CO-COMPLEX OF INOSINE 5'-MONOPHOSPHATE WITH L-SERINE, $2C_{10}H_{13}N_4O_8P.C_3H_7NO_3.16H_2O$ by Sreya Ghosh, S.Pain, I.Dey, G.Biswas, B.P.Mukhopadhyay and Asok Banerjee* Biophysics Department, Bose Institute, Calcutta 700 054 INDIA

Interactions between protein and nucleic acids are ubiquitous and are of fundamental importance in molecular biology. Till now, the structure of a few protein-nucleic acid co-complexes have been reported at low resolution. There is, therefore, need for elucidation of protein-nucleic acid model interaction at atomic resolution since high resolution precise information of unique, simple nucleotide-amino acid/peptide complexes can throw deeper insight on the general recognition rules involved in those broad range of DNA-protein interactions in the biological systems. Recently, we have been successful in getting the single crystal of the co-complex of Inosine 5'-Monophosphate with L-serine in adequate hydrated environment. The physicochemical and IR spectral investigations have clearly indicated the presence of both the parent molecules in the single crystal with other several hydrogen bonded water molecules. The co-complex has crystallised in space group $P2_1$ with cell dimensions a=8.690(1),b=21.898(2),c=12.378(1)Å and ß=110.59(3)° respectively. The structure has been solved by direct methods and the water molecules have been located from the successive difference Fourier analysis. The electron density map of the asymmetric unit has clearly shown the complexation of the two Inosine 5'-Monophosphate with one L-serine and sixteen water molecules. The structure has been refined to current R value of 0.11.

The structure consists of polar hydrophilic columns (made up of the phosphate, sugar hydroxyl, serine, and water molecules) parallel to the a-axis, surrounded by hydrophobic columns (generated by the stacking of the nucleotide bases). An intricate network of hydrogen bonding among the serine groups, nucleotides, and water molecules are present in the structure. The phosphate, 2'- and 3'-hydroxyl, and keto-oxygens (O6) as well as the purine nitrogen (N7) of the nucleotide molecules are involved in the H-bonding scheme with the serine molecules through phosphate oxygens... amino and 2'-hydroxyl...carboxyl groups. Strong H-bonding is observed involving the water molecules themselves and their participation with serine and the nucleotide functional moieties in the hydrophic zones or channels. This structure may suggest some plausible rationale for the interaction of proteins and nucleic acids in the biological system.

PS-04.02.11 AMBIGUOUS PACKING OF DNA HELICES IN CRYSTALS OF d(CGCACG).d(CGTGCG). By C. Sadasivan and N. Gautham, Department of Crystallography and Biophysics, University of Madras, Guindy Campus Madras-600 025, India.

DNA oligomers are known to pack in a few well recognised patterns in single crystals. We report here an unusual space group ambiguity in the crystals of the non-selfcomplementary duplex d(CGCACG).d(CGTGCG) grown from a drop containing 1mM DNA, 50mM sodium cacodylate at pH 6.8, 10mM $BaCl_2$, equilibrated by the hanging drop method against 25% MPD. The X-ray diffraction pattern from a crystal of size 0.2x0.2x0.5 mm was ambiguous and indicated that the X-ray pattern could be indexed in all the space groups given in table 1. All of them can be approximately explained by the same packing mode, viz, that of hexamer duplexes stacked on top of each other in infinitely continuous Z-DNA helices. A continuous helix can be formed by the repetition of two types of arrangement
1) (CGCACG CGCACG).(CGTGCG CGTGCG) and
2) (CGCACG CGTGCG).(CGCACG CGTGCG). In case 1, one hexamer duplex is related to the other by a 2_1 screw along the longest axis, while both the arrangements can give a disordered 6_1 screw, with a dinucleotide duplex as the asymmetric unit. Disordering arises because of the absence of every 6th phosphate group as well as the presence of a T-A base pair instead of C-G base pair. This symmetry is revealed by the systematic absences occuring in data set 1. Similar sequences have been crystallized in space group $P2_12_12_1$. For the same packing, a suitable selection of the unit cell will yield the cell parameters shown in the data set 2. The systematic absences of these data showed the presence of three mutually perpendicular 2_1 screw axes and a C-centering. The volume of the unit cell does not permit a C-centered orthorhombic cell. Therefore, the space group can either be $P2_12_12_1$ or C2. In the case of $P2_12_12_1$, a full turn of helix could be formed as shown in arrangement 1, while arrangement 2 can yield C2. The $R_{(merge)}$ showed more or less equal but unconvincing possibilities for all the four space groups. Therefore, a constrained refinement has been carried out in the space group P1. Present R factor is 0.22 for 612 reflections of $I>3\sigma(I)$ within the resolution limit 7 to 3 Å

Table 1.

	CELL	ABSENCES	SPACE GROUP	R (MERGE)
Set 1	a=17.67 b=17.66 c=42.65 α=90.2 β=89.9 γ=119.9	0 0 1, l≠6n	P61	0.18
			P21	0.22
Set 2	a=17.67 b=30.60 c=42.65 α=90.0 β=90.0 γ=90.0	h 0 0, h=2n+1 0 k 0, k=2n+1 0 0 1, l=2n+1 h k 1, h+k=2n+1	P212121	0.21
			C2	0.22

