respective occupancies and B values of 45%, 23.7Å² and 27%, 12.2Å² bound in regions of the molecule other than the active site. Also, there is an undefined large peak in the electron density map near SG of Cys 212 residue.

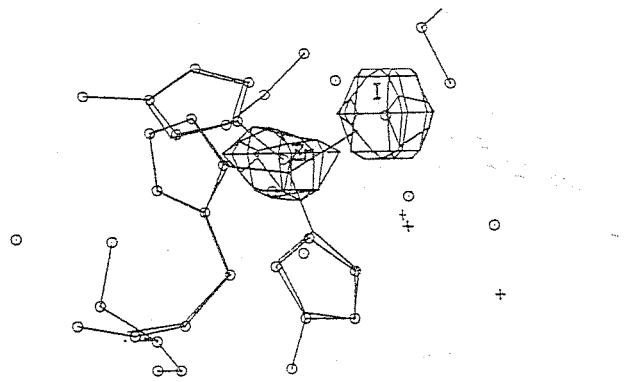

FIG. 1. Zn^{2+} AND I^- IN THE ACTIVE SITE OF HCAI

02.1-21 STRUCTURAL FLEXIBILITY IN RIBONUCLEASES. By L. Mazzarella, S.Capasso, C.A. Mattia, G. Di Lorenzo and A. Zagari, Dipartimento di Chimica, Università di Napoli, Italy.

The structure of bovine seminal ribonuclease (RNAse BS) (Mazzarella, Capasso, Di Lorenzo, Mattia *Gazz.Chim.It.* in press), a dimeric covalent protein strictly homologous to the bovine pancreatic enzyme (RNAse A), has been refined at 2 Å resolution to a final R factor of 0.205 based on 14300 reflections with $I > \sigma(I)$ (≈ 80 % of the total). The final model includes all the non-hydrogen atoms of the two subunits, related by a local twofold axis, 6 sulphate anions and 135 water molecules. The outstanding features of the model are: a) the sixteen-membered cycle linking the two subunits and involving residues Cys30 and Cys31 of the two chains; b) the two active sites formed by residues belonging to different chains. The twofold simmetry is well preserved throughout the structure, but marked deviations are observed for the hinge peptide (residues 15-21) and the external loop (65-72). In the last case the differences are propagated to the two active sites : in one subunit the aspartate 121 is hydrogen bonded to His 119 , whereas in the other subunit it is bonded to the main chain NH group of lysine 66. In both subunits the side chain group of His 119 has been treated as a mixture of two different specific conformations. The structural features in the region of the active sites permitted us to implement the widely accepted mechanism of action of ribonucleases.

02.1-22 THREE-DIMENSIONAL STRUCTURE OF GUANYL-SPECIFIC RIBONUCLEASES FROM MICROORGANISMS AT HIGH RESOLUTION. By B.K. Vainshtein, A.G. Pavlovsky, K.M. Polyakov, S.N. Borisnova, B.V. Strokopytov, A.A. Vagin, Institute of Crystallography, USSR Academy of Sciences, Moscow, USSR.

The crystal structure of guanyl-specific ribonucleases - enzymes catalyzing cleavage of a single-stranded RNA at 3'-phosphodiester bonds of guanyl nucleotides has been studied by X-ray diffraction. Two crystalline modifications of RNase C_2 produced by microfungi of the Asp.-clavatus type have been obtained: the first belongs to space group $P2_1$, a=31.5, b=51.0, c=57.3 Å, γ=92°, 2 molecules per asymmetric unit; the second to space group $P2_1$, a=30.9, b=32.2, c=49.7, γ=116°, 1 molecule per asymmetric unit. Isomorphous replacement was used to solve the structure of the 1st type, whereas the structure of the 2nd type was solved by molecular replacement method and refined to 1.35Å, R=0.198. To solve the crystal homologue structure of RNase Th_1 (Trichoderma harzianum), space group $P3_221$, a=b=55.7, c=80Å, 1 molecule per asymmetric unit, and RNase Pb_1 (Pen.-brevicompactum), space group I222, a=97.8, b=51.7, c=33.9Å, 1 molecule per asymmetric unit, molecular replacement based on the RNase C_2 model was used. The RNase Pb_1 structure was refined at a resolution of 1.75Å, R=0.167.

Isomorphous replacement method was employed to determine the 1st-type structure of the bacterial RNase Bi (Bac.-intermedius); space group B2, a=114.5, b=78.9, c=33.3Å, γ=119°, 2 molecules per asymmetric unit, whereas the 2nd-type structure was determined by molecular replacement: space group $P2_12_12_1$, a=111.4, b=69.6, c=33.5Å, 2 molecules per asymmetric unit. The 2nd-type structure of RNase Bi was refined to 2Å resolution, R=0.21.

Crystalline complexes of RNase Pb_1 with guanosine-3',5'-diphosphate (pGp) (1.24Å resolution, R=0.196) and guanylyl-3',5'-uridine phosphonate analogue were obtained and studied. As a result, a hypothesis was advanced to account for the high specificity of ribonucleases of this type to guanyl bases.

The data on the structure of the RNase Pb_1 complex with pGp gave an insight into the structure of the active site of RNase Bi; in the active site of RNase Bi a region was discovered hypothetically responsible for the recognition of the guanyl base. A comparison of this region with a "recognizing" region in the Pb_1 ribonuclease revealed their close similarity and allowed these two structures to be superimposed. As a result, the nucleotide (pGp) was located in the active site of RNase Bi, thus a "theoretical" complex of this enzyme with a nucleotide was obtained.

The structures of RNase C_2 and Pb_1 were compared.