shown in the Figure. The overall dimensions of the molecule are approximately 33 x 39 x 34 Å. The shape and dimensions are listed in the Table. The structure of cytochrome C3 from D. desulfuricans, which has been reported by Basu et al., has not been included because their structure was not possible. It seems that the peptide backbone of these two proteins differs significantly. This would be the case if the cytochrome C3 family proteins became available.

<table>
<thead>
<tr>
<th>Distance (Å)</th>
<th>Heme</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heme-Heme Distances (upper right) and (lower left)</td>
<td>3</td>
<td>22</td>
<td>89</td>
<td>11.3</td>
<td>-</td>
</tr>
<tr>
<td>Heme-Heme Angles</td>
<td>4</td>
<td>80</td>
<td>64</td>
<td>82</td>
<td>-</td>
</tr>
</tbody>
</table>

02.1-22 CRYSTAL STRUCTURE DETERMINATION OF A DD CARBOXYPEPTIDASE AT 2.5 Å RESOLUTION.

The exocellular DD-carboxypeptidase of Streptomyces albus G is a metallo (Zn++) enzyme. The cofactor is required for activity on substrates analogues (e.g., Ac-G.Lys-D-Ala-D-Ala) and for binding of S-lactam antibiotics. We have obtained a 2.5 Å resolution map using the method of multiple-isomorphous replacement supplemented by anomalous-scattering information. Three heavy-atom derivatives were used: K₄AuCl₆, K₃UO₆F and K₃Pt(CO)₆. For 6,700 reflections the figure of merit was 0.55. The electron density map allowed a tracing of almost all the polypeptide chain. The molecule is divided into two domains. The smallest one (71 residues) consists of three helices and random coil regions. The other domain (105 residues), where the zinc ion (catalytic site) is located, consists of two parallel strands and two α-helices, and possesses the only two disulfide bridges. No conformational similarities exist between this DD-carboxypeptidase and other Zn++ metallo-enzymes such as carboxypeptidase A and thermolysin. Ligand binding studies and high resolution map are currently under investigation, details and implications of the protein-drug interactions will be reported.

02.1-23 X-RAY CRYSTAL STRUCTURE OF A PENCILLIN TARGET: STREPTOMYCINES R61 DD-TRANSPEPTIDASE-CARBOXYPEPTIDASE.

The DD-transpeptidase-carboxypeptidase from S. R61 is an exocellular, penicillin sensitive enzyme (MW 38,000 daltons). The reactions catalyzed are:

\[
\text{Penicillin} \rightarrow \text{D-Ala-D-Ala} \rightarrow \text{acyl penicillin} \rightarrow \text{penicillin}
\]

These reactions are crucial in the growth and maintenance of the bacterial cell wall and are inhibited by beta-lactam antibiotics. The crystal structure of this enzyme is being determined in order that we may visualize its interactions both with cell-wall substrates and with beta-lactam inhibitory molecules.

The crystals of the DD-transpeptidase are orthorhombic (P2₁2₁2₁) with unit cell dimensions a = 51.1, b = 67.5 and c = 102.9 Å (Phil. Trans. R. Soc. Lond. B 282, 361 (1980); J. Molec. Biol. 125, 217 (1979)). The structure has been solved to 2.9 Å resolution using three heavy atom derivatives, Na₃PtCl₆, K₃UO₆F and CH₃HgCl. The binding site of ortho-iodosphenylpenicillin has been located in a well-defined cleft in the molecule.

Supported by grant AI-16702 from the NIH.