

E0013

A Problematic Case: Crystal Structure of Disintegrin Using Data from a Crystal with Pseudosymmetry. Sameeta Bilgrami¹, P. Kaur¹, S. Yadav¹, A.S. Ethayathulla¹, R. Prem Kumar¹, T. Jabeen¹, S. Sharma¹, M. Perbandt², Ch. Betzel², T.P. Singh¹, ¹Dept. of Biophysics, All India Inst. of Medical Sciences, New Delhi, India, ²Inst. of Medical Biochemistry and Molecular Biology, c/o DESY Notkestrasse 85, Hamburg, Germany.

Disintegrins constitute a family of potent polypeptide inhibitors of integrins and have shown great potential as anticancer and antithrombotic agents. A novel homodimeric disintegrin has been isolated from the venom of saw-scaled viper (*Echis carinatus*) having a molecular weight of 14 kDa. The X-ray intensity data were collected on consortium beamline X-13 at DESY, Hamburg. The crystals diffracted upto 1.9 Å resolution and apparently belonged to the space group P4₃2₁2 with cell dimensions of a = b = 90.2 Å, c = 54.7 Å. Further examination of the diffraction pattern indicated that the reflections corresponding to the condition of h + k + l = 2n + 1 were systematically weak. The native Patterson calculated using data to 3.0 Å resolution gave an off origin peak at 0.5, 0.5, 0.5 which was about 70% of the origin peak suggesting a high level of pseudosymmetry. As 50% of all the data were weak, molecular replacement failed to give a solution in the primitive lattice, even though the model used was that of the previously solved dimer of disintegrin at 2.5 Å resolution. In order to identify the correct space group with the primitive cell the origin shifts were applied to the dimer solved earlier at 2.5 Å in space group I4₁22 with similar cell dimensions. These origin shifts were refined in AMoRe with fitting against the weak data corresponding to h + k + l = 2n+1 reflections. The structure finally refined in the space group P4₃2₁2 to a final R_{cryst}/R_{free} of 21.5/25.5 with good geometric parameters.