

W0431

A Comparison of Pt and Br Phasing for Structure Determination.[‡] B.D. Santarsiero^{*}, K. Ratia^{*}, K.S. Saikatendu[§], N. Barretto[†], S.C. Baker[†], R.C. Stevens[§], A.D. Mesecar^{*}, ^{*}Center for Pharmaceutical Biotechnology and Dept. of Medicinal Chemistry and Pharmacognosy, Univ. of Illinois at Chicago, Chicago, IL 60607; [§]Depts. of Cell and Molecular Biology, The Scripps Research Inst., [†]Dept. of Microbiology and Immunology, Loyola Univ., Chicago Stritch School of Medicine.

We have determined the structure of PLpro, a SARS coronavirus papain-like protease, to a resolution of 1.85Å. The native enzyme, with 313 residues, crystallizes in space group C2 with three chains related by non-crystallographic symmetry. We obtained two heavy atom derivatives using Pt and Br. The Pt derivative was collected at one wavelength, and the Br derivative was collected at two different wavelengths. All three data sets, and a native data set, were used for initial phasing using SOLVE. Six Pt atoms but no Br atoms were found. HYSS finds five Pt atoms or six Br atoms from their respective data sets. The Br data is at the highest resolution, and we used one of the data sets for building and refinement of the structure; nine Br atoms are included in the final model. This affords an opportunity to compare the phasing power of Pt vs. Br. We also compare the different results in phasing using SOLVE, HYSS, and other phasing programs.

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