A resolution with R-merge 5.7, mosaicity 0.295 and completeness 86.9%. On the other hand, L-PGDS crystals were previously obtained with citrate as a precipitant and diffracted to 2.0 Å (PDB ID: 2CZT). In microgravity, we obtained L-PGDS crystal which diffracted up to 1.0 Å resolution with R-merge 0.064, mosaicity 0.16 and completeness 98.8%.

References

Keywords: atomic resolution crystallography, inhibitor and drug design, microgravity crystallization

**P04.23.442**

*Acta Cryst. (2008).* A64, C368

**Protein helix-dipole calculations based on experimental electron densities**

Dorothee C. Liebschner, Benoît Guilhot, Christian Jelsch, Claude Lecomte
Faculté des Sciences et Techniques, LCM3B, BP 239, Boulevard des Aiguillettes, Vandoeuvre-lès-Nancy, Lorraine, 54506, France, E-mail: dorothee.liebschner@lc3b.ups-nancy.fr

Since the 1970’s, it has been assumed that the alpha helix represents a macro dipole. This is due to the dipole moment of the individual peptide units, which are aligned parallel to the helix-axis and thus form a macro-dipole. The helix-dipole is guessed to have effects upon the functioning and structure of proteins [1]. However, the exact dipole strength is still unclear. Estimations include only the atomic charges of the main chain and not of the side chains. Dielectric measurements of the dipole strength using helical oligopeptides in solution have been made [2], but lack of precision as the percentage of the peptides with helical conformation is unknown. Here, we propose an estimation of the alpha-helix-dipole referring to experimental electron density distributions. The electron density of isolated amino acid compounds has been refined with the program MoPro (Molecular Properties, [3]) using the Hansen and Coppens multipole formalism [4] to create an experimental electron density distribution database (ELMAM, [5]). The atomic charges described in the ELMAM database are then transferred to the protein. The dipole moment of the alpha-helix is calculated either by using the transferred charges or, if the protein diffracts at subatomic resolution below 0.8 Å, by using charges that are refined against X-ray diffraction data.


Keywords: helix-dipole, subatomic resolution, electron deformation density

---

**P04.23.443**

*Acta Cryst. (2008).* A64, C368

**Charge density analysis of human aldose reductase active site**

Benoit Guilhot¹, Christian Jelsch¹, Alberto Podjarny², Claude Lecomte¹
¹LCM3B, Faculté des Sciences et Techniques, Vandoeuvre-lès-Nancy, France, 54506, France, ²JGBMC, Structural Biology and Genomics Department, Strasbourg, France, E-mail: benoit.guilhot@lc3b.ups-nancy.fr

Human aldose reductase (hAR) is a NADPH dependent enzyme involved in diabetes complications. Crystals of hAR in complex with NADPH and the Idd594 inhibitor diffract up to 0.66 Å resolution [1]. Such subatomic resolution X-ray data allows, after a restrained IAM refinement, the observation of significant residual deformation electron density on covalent bonds. This residual electron density peaks are the deviation from the spherical approximation of the atomic electron clouds, due to chemical bonding. The Hansen & Coppens [2] multipolar model, implemented in the MoPro [3] software, allows taking into account the deformation electron density. Hence a constrained multipolar refinement of hAR has been performed, leading to decreased atomic thermal motion amplitudes and better stereochemistry [4]. Here we present the continuation of this work: a precise, unconstrained, charge density analysis focusing on hAR active site. Deformation electron densities of the NADPH cofactor, the Idd594 inhibitor and the catalytic amino acids have been modelled using the multipolar formalism. Then a topological analysis of hAR active site electron density has been performed in order to derive informations related to the inhibitor binding and the catalytic mechanism.


Keywords: charge density, high-resolution crystallography, protein ligands

---

**P04.23.444**

*Acta Cryst. (2008).* A64, C368-369

**Ultra-high resolution structure of endopolygalacturonase determined by X-ray and neutron diffraction**

Tetsuya Shimizu¹, Toru Nakatsu², Nobutaka Shimizu²,³, Mamoru Sato, Kazuo Kurihara², Kazuo Miyairi², Toshikatsu Okuno³, Nobuo Niimura³, Masaki Yamamoto²,³, Hiroaki Kato²
¹RIKEN SPring-8 Center, Division of Synchrotron Radiation Instrumentation, 1-1-1, Kouto, Sayo-cho, Sayo-gun, Hyogo, 679-5148, Japan, ²RIKEN, SPring-8 Center, 1-1-1, Kouto, Sayo-cho, Sayo-gun, Hyogo, 679-5148, Japan, ³Spring-8/JASRI, 1-1-1, Kouto, Sayo-cho, Sayo-gun, Hyogo, 679-5148, Japan, ³Graduate School of Integrated Science, Yokohama City University, 1-7-29 Suehirocho, Tsurumi-ku, Yokohama 230-0045, Japan, ⁴JAEA, Tokai, Ibaraki 319-1195, Japan, ⁵Faculty of Agriculture and Life Sciences, Hirosaki University, 3 Bunkyo-cho, Hirosaki, Aomori 036-8561, Japan, ⁶Graduate School of Science and Engineering, Ibaraki University, 2-1-1 Bunkyo, Mito, Ibaraki 310-8512, Japan, E-mail: shimizu@spring8.or.jp

Endopolygalacturonases (endoPGs) are inverting glycosidases that...