MS42-P3 **Zn(II) coordination in human and bovine bromo- and iodo-insulin hexamers.** Dubravka Matković-Čalogović, Biserka Prugovečki and Ivica Đilović
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The insulin hexamer is an allosteric protein that exists in three conformational states: T_6, $T_3R_3^f$ and R_6 [1]. Transitions between conformational states are mediated by the binding of phenolic compounds or by the coordination of anions to the bound metal ions [2-5]. It was found that $T_3R_3^f$ hexamer in the chloro-derivative can accommodate different number of Zn^{2+} ions per hexamer with different coordination of the zinc ion [4,5].

In the present study four new insulin derivatives (two human and two bovine) crystallized in the presence of bromide or iodide ions and were structurally characterized. Single crystal diffraction data at 100 K were collected to high resolution at synchrotrons ELETTRA and ESRF.

In the bromo-derivatives four different coordinations of the Zn^{2+} ion were found: i) tetrahedral with two histidines and two bromide ions, ii) disordered site – tetrahedral with three histidines and one bromide ion and – octahedral with three histidines and three water molecules and; iii) tetrahedral tetraaquazinc(II) ion which was not found in the published chloro-derivatives and is rarely found in small molecule crystal structures. All bromo-derivatives are of the $T_3R_3^f$ type.

In the iodo-derivative only the ii) type of the disordered octahedral-tetrahedral site is found. The human bromo-derivative is a superstructure with a doubled *c*-axis. This derivative is also $T_3R_3^f$ but is of the 2Zn type with Zn^{2+} ions only on the three-fold axis.

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Keywords: insulin; bromine; iodine

MS42-P4 **Multipolar refinement of amino acids with anisotropic H atoms treatement.** Aleksandra Pazio[a], Matthias Gutmann[b], Paulina Dominiak[a], Krzysztof Woźniak[a*], [a]*Department of Chemistry, Warsaw University, Warsaw, Poland*; [b]*ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, UK*
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The high resolution X-ray diffraction experiments have been conducted by different research groups on 12 amino acids only, all studies were performed in different conditions and using several types of radiation source (MoKα, AgKα, synchrotron radiation). Moreover, hydrogen atoms were treated in various way depending on a research group involved in such studies. Testing the best way of obtainig proper anisotropic displacement parameters for amino acids we have made a comparison of the multipole refinements, conducted for selected amino acids, with the anisotropic H atoms treatement.

(a) using the SHADE server (Madsen, 2006) which provides an estimated anisotropic displacement parameters for H atoms (Fig.1A),
(b) using data obtained from the single-crystal neutron diffraction measurement on VIVALDI in ILL, Grenoble, France (Fig.1B),
(c) using data obtained from the single-crystal neutron diffraction measurement on SXD in ISIS, Chilton, UK (Fig.3C).

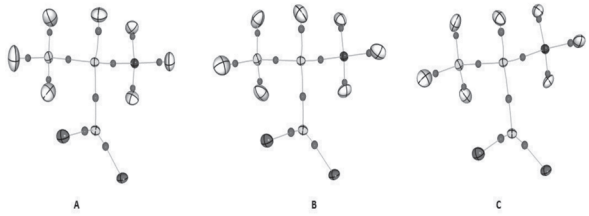

Fig. 1 Anisotropic displacement parameters, bond paths and bond critical points of l-alanine refined on three sets of data: (A) SHADE (B) ILL (C) ISIS.

The obtained results shows no significant differences between three models and the R-factors at the end of the refinement.

Keywords: charge density, amino acids