Charge Density of two Dipeptides from Fast Synchrotron/CCD Area Detector Experiments

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In our program of comparative charge density studies on biologically important molecules we have directed our interest from amino acids to oligopeptides. Recently we have investigated the dipeptide glycyl-L-threonine [1] and the hexapeptide cyclo-L-Ala_4-L-Pro_2. Studies with synchrotron radiation at low temperature have proven to be an excellent tool to obtain precise information about the electron density distribution (EDD) [2]. The evaluation of the EDD with the AIM-Formalism of R.F.W. Bader [3] furthermore allows to obtain and compare quantitative results, i.e. the electron density ρ, the Laplacian $\nabla^2\rho$ or the bond ellipticity ϵ at the bond critical point (bcp). Our interest in this field of research is to analyze the degree of transferability from bonds or functional groups from amino acids and oligopeptides to larger peptides based on experimental results using the Bader formalism. Results from studies of several amino acids [4] have shown, that there is a high similarity between chemically equivalent bonds within this class of molecules. The difference between amino acids, that have, apart from the rest R, the same functional groups at the Cα carbon atom, and oligopeptides is the peptide bond. To adress the question of transferability the dipeptides

molecule	L-Arg-L-Glu · 4 H_2O	L-His-L-Ala · 2 H_2O
fromula	$C_{11}H_{21}N_5O_5$ · 4 H_2O	$C_9H_{13}N_4O_3$ · 2 H_2O
crystal system	orthorhombic	monoclinic
beamline	F1	D3
wavelength	0.5503	0.5611
max. resolution		
d	0.38	0.40
sin θ/λ	1.30	1.26
temperature	100 K	100 K
no. of reflections:		
total measured	69855	31726
unique	14095	9690
used($>2.5\sigma$	10902	8785
R(F)	0.035	0.030
Rw(F)	0.032	0.028

Table 1: Experimental and crystal data, figures of merit

L-Arg-L-Glu tetrahydrate and L-His-L-Ala dihydrate were measured. Two high resolution single crystal experiments at a temperature of 100 K with synchrotron radiation with short wavelengths and CCD area detection were carried out. The datasets were analyzed with the program package XD [5] that allows a multipolar refinement [6] and a topological analysis of the charge density. Table 1. shows information about the experiments and the figures of merit.

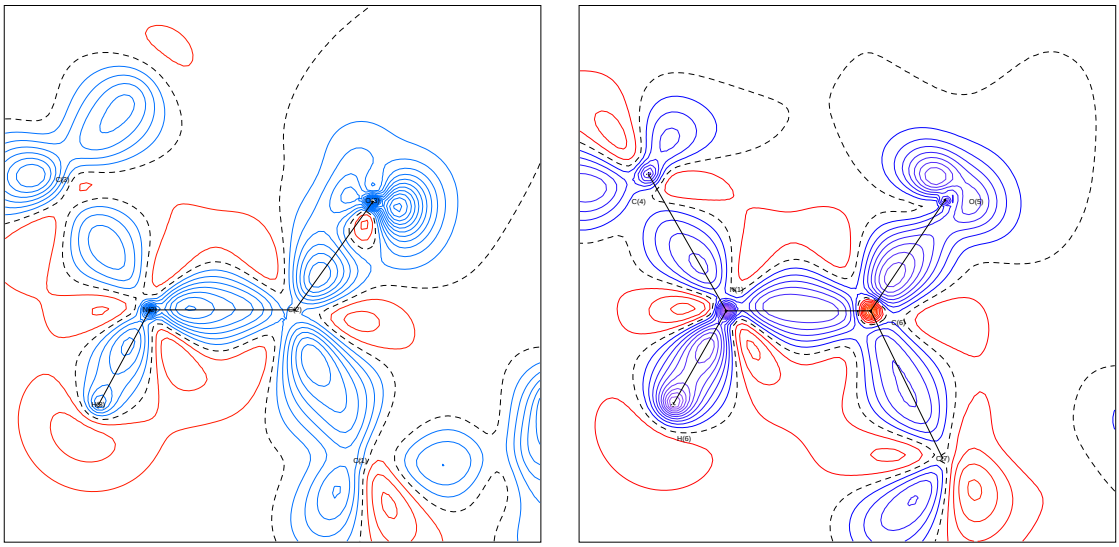

Figure 1: Deformation density in the plane of one peptide groups

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