

## Supplementary information:

A CSD [1] search using version 5.27, including updates from August 2006 and excluding complexes with metals, gave the following structures containing the ornithine fragment. These are L-ornithinium sulfate monohydrate [2], L-ornithine L-aspartate hemihydrate [3], bis(L-ornithinium) chloride nitrate sulfate [4], L-ornithine aspartate monohydrate [5] DL-ornithine hydrobromide [6, 7], a second determination of L-ornithine hydrochloride [8], L-ornithine nitrate [9], L-ornithine dipicrate [10] and L-ornithine aspartate monohydrate [11].

Figures 1-5 show static deformation density plots of the experimentally determined and the invariom-database electron density as well as residual electron density maps for these two models and additionally the independent atom model using all data in each case.

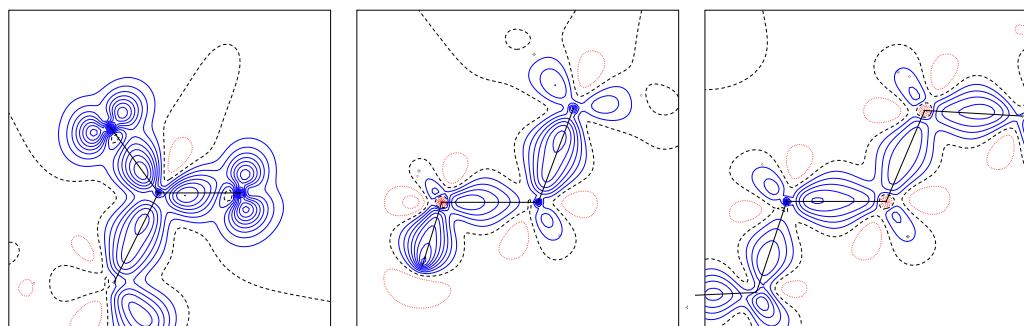


Figure 1: Static deformation density of the experimental charge density refinement in the plane of the carboxylate group, the N1C2C1 plane and the C2C3C4 plane; contour lines with  $0.1 \text{ e}\cdot\text{\AA}^{-3}$  steps, blue = positive, red = negative, zero contour dashed.

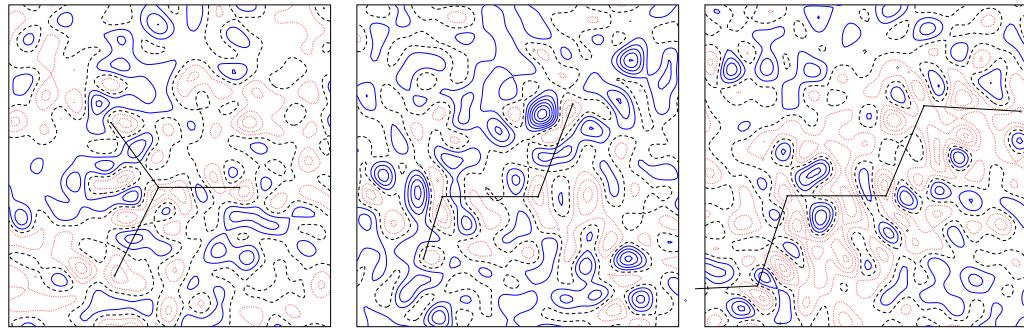


Figure 2: Fourier residual density map of the experimental charge density refinement in the plane of the carboxylate group, the N1C2C1 plane and the C2C3C4 plane; contour lines with  $0.05 \text{ e}\cdot\text{\AA}^{-1}$  steps, blue = positive, red = negative, zero contour dashed.

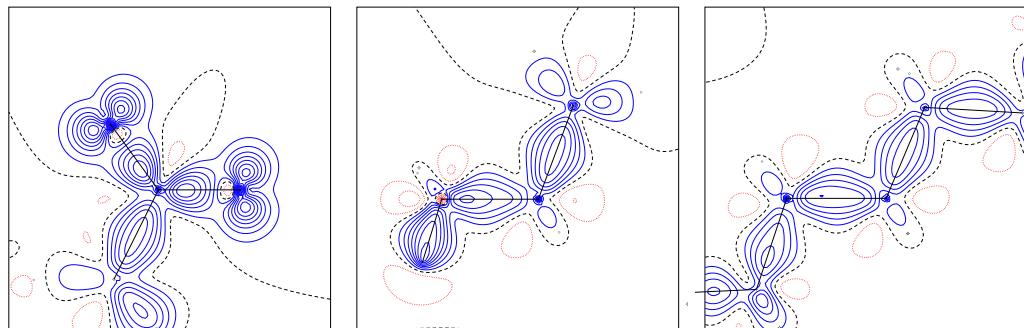


Figure 3: Static deformation density of the invariom model refinement in the plane of the carboxylate group, the N1C2C1 plane and the C2C3C4 plane; contour lines with  $0.1 \text{ e}\cdot\text{\AA}^{-1}$  steps, blue = positive, red = negative, zero contour dashed.

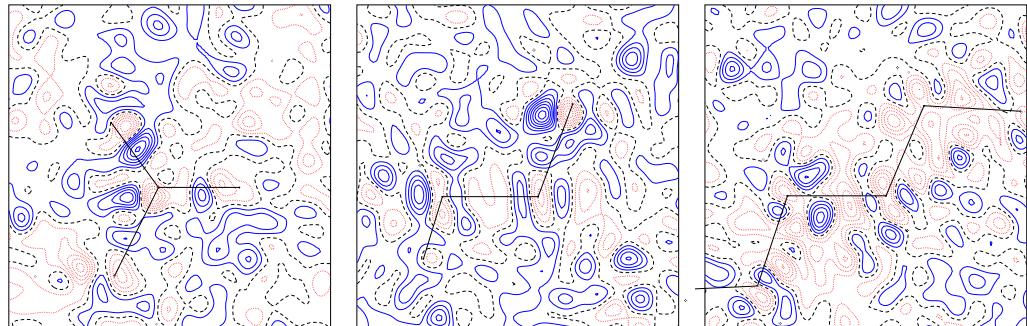


Figure 4: Fourier residual density map of the invariom model refinement in the plane of the carboxylate group, the N1C2C1 plane and the C2C3C4 plane; contour lines with  $0.05 \text{ } e\cdot\text{\AA}^{-1}$  steps, blue = positive, red = negative, zero contour dashed.

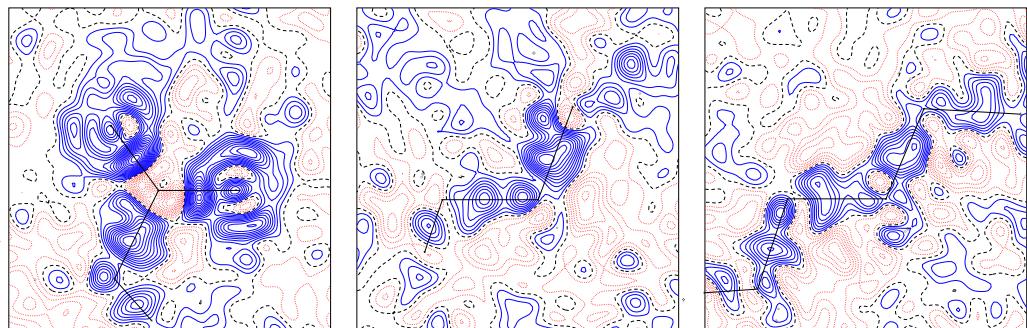


Figure 5: Fourier residual density map of the independent atom model refinement in the plane of the carboxylate group, the N1C2C1 plane and the C2C3C4 plane; contour lines with  $0.05 \text{ } e\cdot\text{\AA}^{-1}$  steps, blue = positive, red = negative, zero contour dashed.

## References

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