## Supplementary information:

Figure 1 shows a static deformation density plot of the invariom-database electron density.  $\,$ 

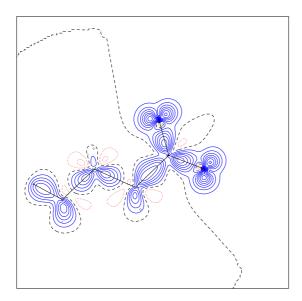


Figure 1: Static deformation density of the predicted charge density in the molecular plane of sarcosine calculated using N1 O1 and O2; contour lines with  $0.1~e\cdot {\rm \AA}^{-1}$  steps, blue = positive, red = negative, zero contour dashed.