



JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

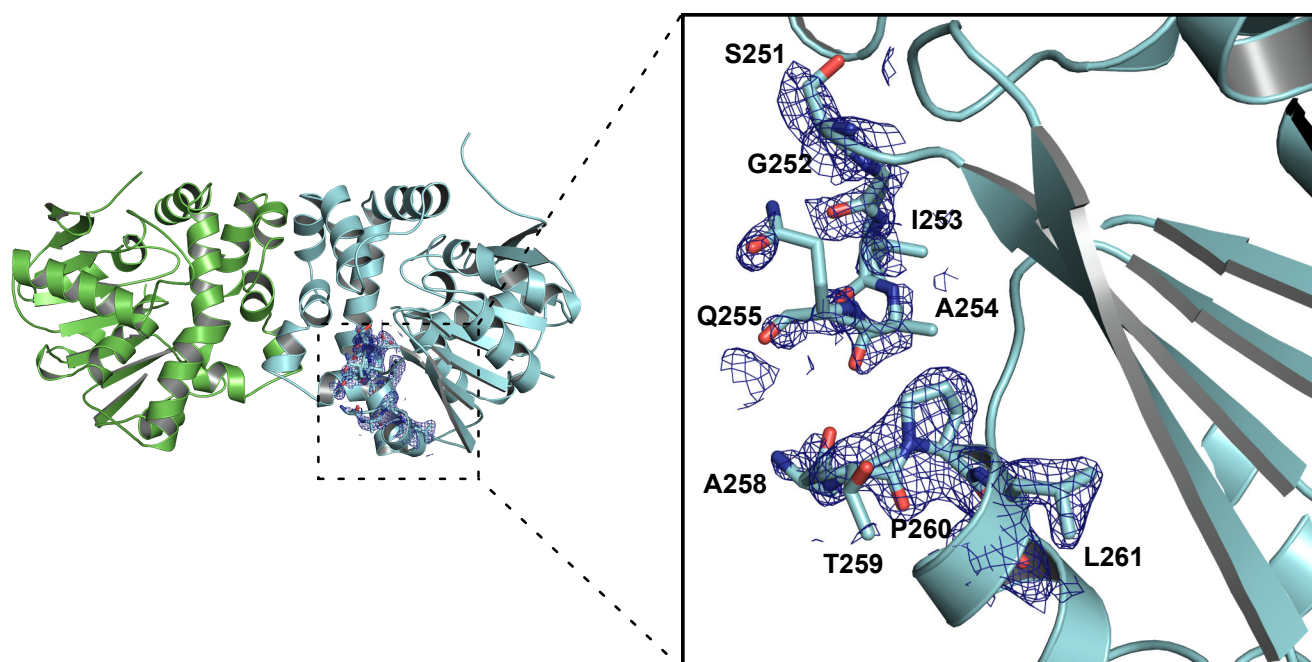
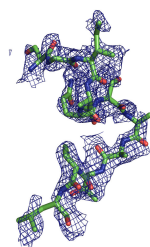
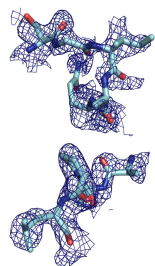
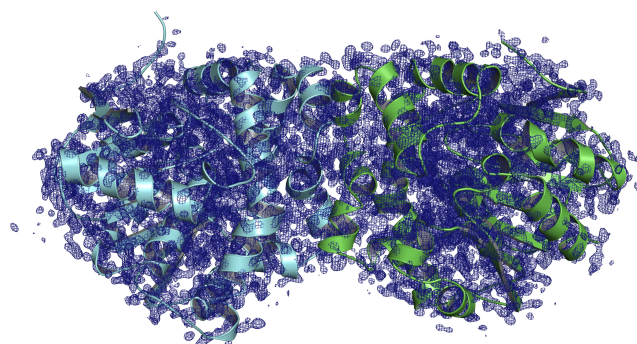
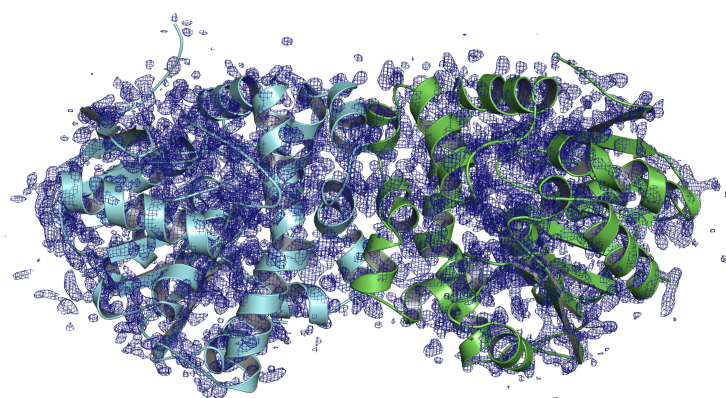
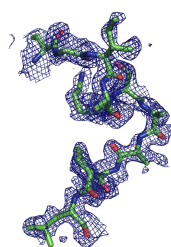
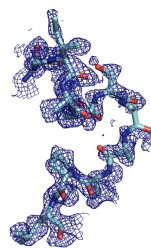
Volume 50 (2017)

Supporting information for article:

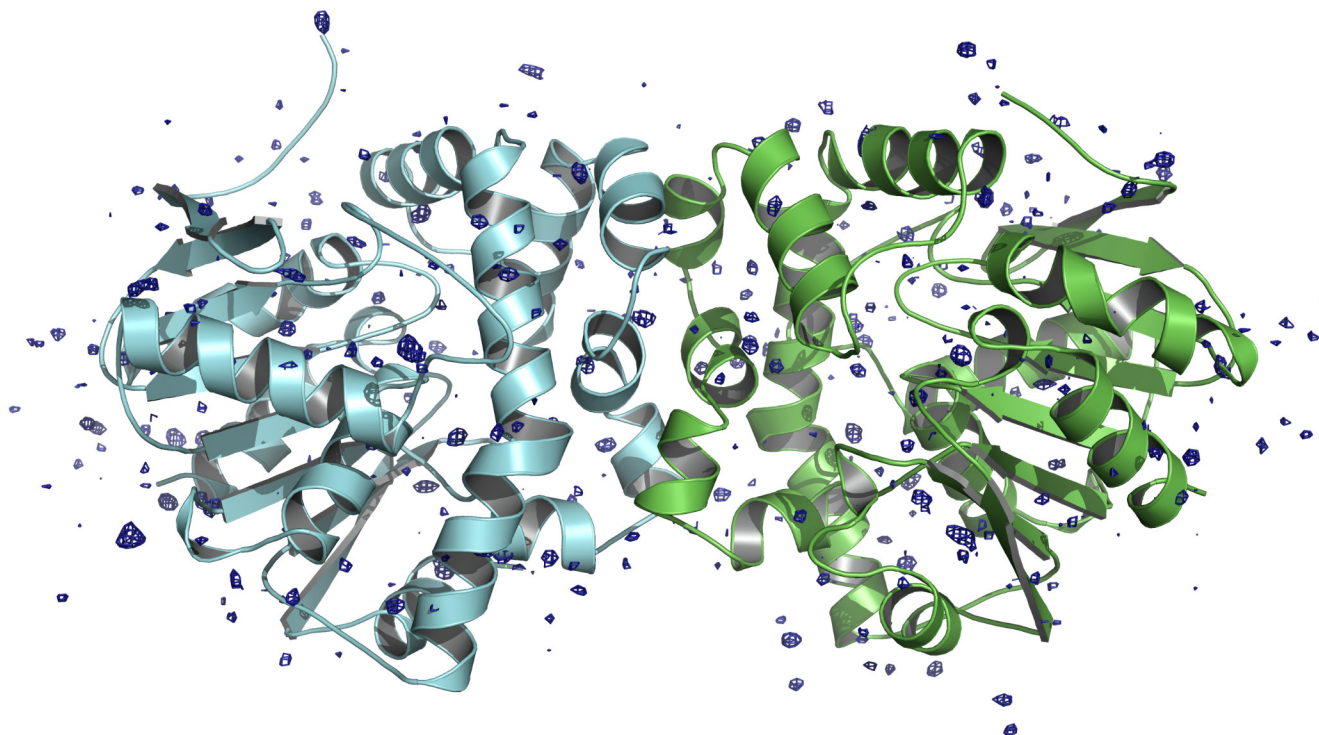
Protein crystals ablated from aqueous solution at high velocity retain their diffractive properties: applications in high-speed serial crystallography

Eike C. Schulz, Johannes Kaub, Frederik Busse, Pedram Mehrabi, Henrike M. Müller-Werkmeister, Emil F. Pai, Wesley D. Robertson and R. J. Dwayne Miller

Supplementary Figure 1 Crystal structure of the PIRL-ablated FAcD. The overview image shows the two FAcD subunits in cyan and green. **A)** A simulated annealing omit map is shown for residues B251-B261 at the 1 sigma level. The simulated omit map shows backbone density for the region with the exception of residues 256 and 257, which were not included in the final PIRL model. **B)** A composite simulated annealing omit map is shown at the 2 sigma level for the overview panels and at the 1 sigma level for the details. The maps show continuous backbone density for residues 251-261 of chain A (green) in the control data as well as in the PIRL data. The same region has weaker density for residues 256 and 257 in chain B in the control data and is absent in the PIRL dataset.

A**B****PIRL****CONTROL****Chain B****Chain A****Chain B****Chain A**

Supplementary Figure 2 An isomorphous difference map ($|F_{\text{obs}}^{\text{PIRL}} - F_{\text{obs}}^{\text{Control}}|$) between the PIRL dataset and the control dataset was calculated between 50 and 2.1 Å resolution. **A)** Crystal structure of the PIRL ablated FAcD. The overview image shows the two FAcD subunits in cyan and green. An isomorphous difference map is displayed as a blue mesh at the 3 sigma level. Most difference map peaks can be observed in the solvent region or in the proximity of sidechains indicating that the PIRL-ablated structure is comparable to the untreated one. **B)** A plot of the isomorphous difference between 8 and 2.1 Å resolution confirms this observation. While the correlation coefficient (CC_{iso}) measures the agreement, the difference between both maps is shown by R_{iso} . The PIRL dataset is isomorphous to the control dataset up to a resolution of ~2.8 Å.

A**B**