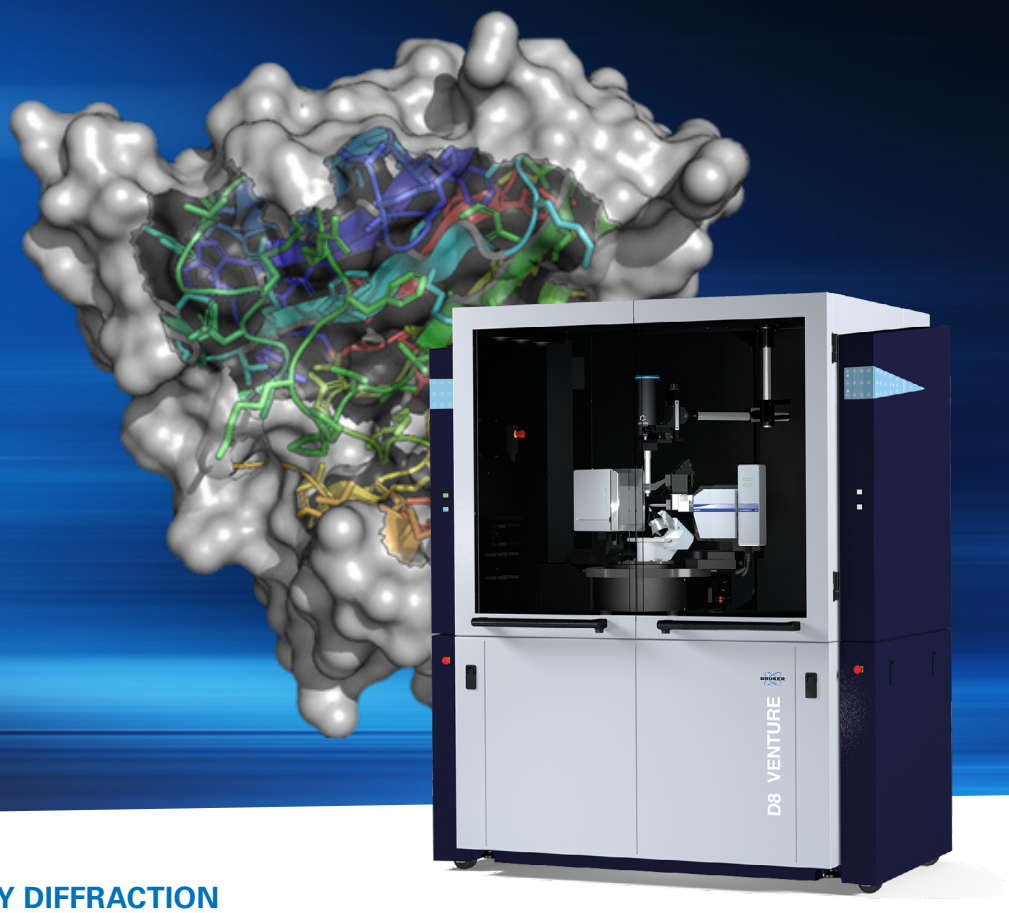

SINGLE-CRYSTAL X-RAY DIFFRACTION

D8 VENTURE with IμS DIAMOND II

1.8 Å high-quality in-house data in less than a minute

Summary

Fast data collection saves you time and resources. Harnessing the new Diamond Hybrid Anode technology the IμS DIAMOND II source delivers a remarkably bright spot and allows you to take full advantage of the high sensitivity of the PHOTON III detector.

This combination of enhanced source intensity and outstanding detector efficiency enables the quick evaluation of crystal quality and fast retrieval of structural information.

The outstanding performance of the D8 VENTURE with IμS DIAMOND II also enables very small crystals to be measured that, until recently, could only be collected on maintenance-intensive rotating anode systems or even required synchrotron usage.

This report highlights the D8 VENTURE performance by solving the structure of the protein thaumatin from *Thaumatococcus daniellii* to 1.8 Å in only fifty-five seconds.

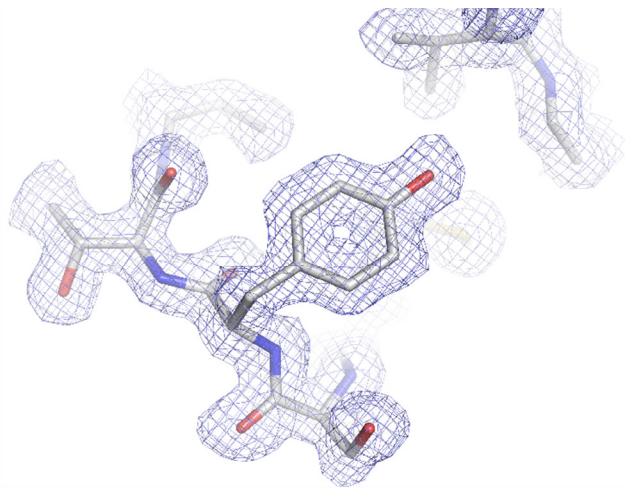

Figure 1
Residue TYR 11 of thaumatin with the electron density map contoured at 1σ.

Table 1

A 1.8 high-quality in-house data in less than a minute

Crystal and Data statistics	
Unit cell	a = b = 57.84 Å c = 150.28 Å
Spacegroup	$P4_12_12$
Resolution	24.46-1.80 (1.84-1.80)
R_{merge}	0.267 (0.501)
R_{meas}	0.298 (0.586)
R_{pim}	0.131 (0.299)
Number of observations • unique	119 463 (4951) 24 533 (1397)
Mean $I/\sigma(I)$	5.6 (2.6)
CC (1/2)	0.97 (0.539)
Completeness [%]	99.9 (99.6)
Multiplicity	4.9 (3.5)

Table 2

PHASER molecular replacement solution

Structure statistics PHASER	
Resolution [Å]	24.46-1.80
No. reflections all/free	24464 / 1269
R-factor/*R*-free	0.256 / 0.277
RMS Deviations:	
Bonds	0.0070
Angles	1.456
Mean Chain B-factors: Chain A [Å²] (#atoms)	7.9 (3103)

References:

[1] Bruker (2022). PROTEUM v.2022.10-0. Bruker, Madison, Wisconsin, USA.

[2] Evans, P.R., & Murshudov, G.N. (2013). *Acta Cryst.* **D69**, 1204-1214.

[3] McCoy, A.J., Grosse-Kunstleve, R.W., Adams, P.D., Winn, M.D., Storoni, L.C. & Read, R.J. (2007). *J. Appl. Cryst.* **40**, 658-674.

[4] Cowtan, K., Metcalfe, S. & Bond, P. (2020). *Acta Cryst.* **D76**, 1192-1200.

[5] Agirre J. et al (2023). *Acta. Cryst.* **D79**, 449-461.

Results

A complete data set was collected in 54.8 sec to a resolution of 1.8 Å. The data statistics are displayed in Table 1. Even though thaumatin crystals have a moderately long axis of 150 Å, the reflections were well separated on the PHOTON III detector at a sample-detector distance of only 45 mm.
The detector's high spatial resolution combined with a large active area make it very easy to acquire complete data sets in ultimately short time. The structure was solved with molecular replacement using PHASER[3]. A quick shift field refinement of the solution produced a R / R_{free} of 25.6 / 27.7% and a very good electron density map (Figure 1). The refinement statistics are presented in Table 2.

Experimental

A crystal of thaumatin (MW 22.4 kDa) with dimensions of 0.160 × 0.280 × 0.340 mm³ was measured on a D8 VENTURE equipped with a IμS DIAMOND II microfocus source (Cu-Kα radiation, λ = 1.54184 Å), PHOTON III 14 detector and KAPPA goniometer at 100 K. The beam divergence was collimated to 7.0 mrad to optimize reflection separation at the detector distance of 45 mm. Complete data were collected using a single omega scan of 68.5°in 54.8 sec. Data collection and reduction were conducted using the PROTEUM[1] software suite, which is included to the instrument. Data statistics were generated using AIMLESS[2]. If CCP4 is installed locally, AIMLESS can be easily run through PROTEUM to generate merging statistics plus a mtz file. The mtz file than can be imported directly into CCP4 or PHENIX. The molecular replacement solution was determined using PHASER and the PDB model (1RQW). Refinement was preformed after the MR run in PHASER[4]. AIMLESS and PHASER were used as part of the CCP4[5] software suite.

Conclusions

- The combination of a very-high intensity IμS DIAMOND II source with the PHOTON III detector enables complete data to be collected in under one minute.
- The large active area and excellent point spread of the PHOTON III allow data to be collected very efficiently at short crystal-detector distances, even when moderately large unit cells are encountered.
- The enhanced performance of the D8 VENTURE produces results, structures, and high-quality electron density maps, that rival or exceed the capabilities of rotating-anodes systems without the maintenance requirements and expense.

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