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AcrB et al.: Obstinate contaminants in a picogram scale. One more bottleneck in the membrane protein structure pipeline

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Table 1

Crystallization conditions for the observed crystals obtained in this work.

Crystallization conditions		Diffraction (Å)
1A	250 mM KCl, 25mM MOPS (pH 7.0), 6% PEG 4000, 10% Glycerol	-
2A	100 mM MgCl ₂ , 50 mM Tris (pH 8.5), 6% PEG 4000	4.20
3A	25 mM HEPES (pH 7.5), 5% PEG 10000, 2% Ethylene glycol	6.4
4A	50 mM NaCl, 50 mM BICINE (pH 9.0), 10% PEG 550 MME	6.7
5	50 mM MgCl ₂ , 50 mM ADA (pH 6.5), 6% PEG 6000	-
6	50 mM (NH ₄) ₂ SO ₄ , 25 mM MES (pH 6.5), 7.5% PEG MME 5000	10.4

Note. The end concentrations in the crystallization drop are provided. Data for the crystallization conditions 1A-4A correspond to the crystals shown in Fig. 2.

Table 2

Crystallographic data processing & refinement

Data collection	AcrB crystal from GluP condition
X-ray source and wavelength	SLS, PX06SA, 0.9000 Å
Detector	MAR CCD 225 mm
Space group	<i>H</i> 32
Unit-cell dimensions (Å)	146.53, 146.53, 515.02
Resolution	35 – 4.2 Å
Observations; unique reflections	66936; 14936
Mosaicity	0.93°
$I/\sigma(I)$; R_{merge}^*	8.8 (1.3); 0.102 (0.561)
Completeness (%)	94.8 (74.6)

$$^* R_{\text{merge}} = \frac{\sum_{hkl} \sum_i |I_i(hkl) - \langle I(hkl) \rangle|}{\sum_{hkl} \sum_i I_i(hkl)}$$

Note. Statistical values in parentheses correspond to the highest resolution shell.

Figure 1

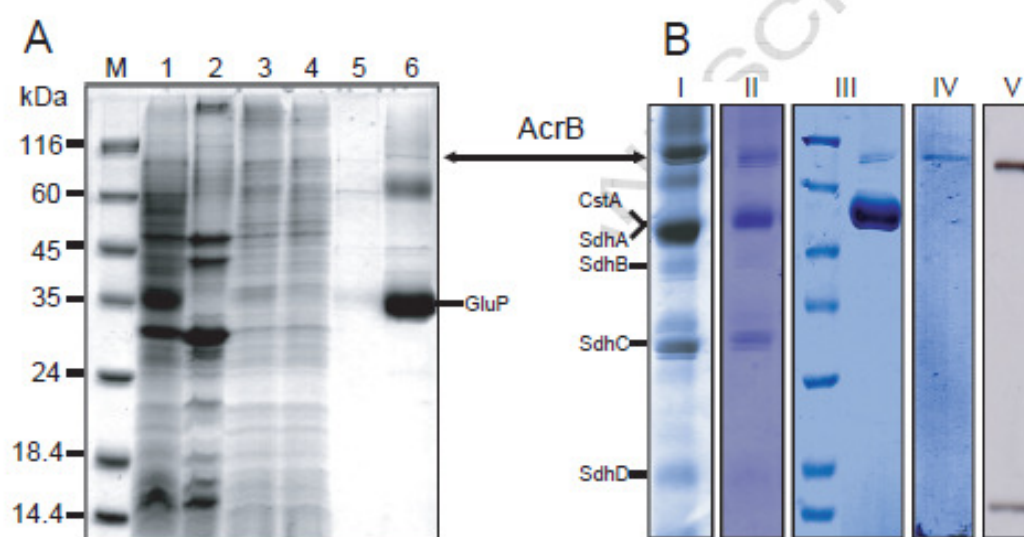


Figure 2

