Table 9. Crystal data and structure refinement for **4**.

Identification code	**4**
Empirical formula	$C_{29}H_{43}BCdN_2S_3$
Formula weight	639.04
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 15.5893(8) Å a= 90°.
	b = 18.0471(9) Å b= 90°.
	c = 22.2133(12) Å g = 90°.
Volume	6249.5(6) $Å^3$
Z	8
Density (calculated)	1.358 Mg/m^3
Absorption coefficient	0.919 mm^{-1}
F(000)	2656
Crystal size	0.30 x 0.20 x 0.10 mm^3
Theta range for data collection	1.83 to 28.34°.
Index ranges	-20<=h<=17, -23<=k<=24, -28<=l<=24
Reflections collected	29757
Independent reflections	7497 [R(int) = 0.0307]
Completeness to theta = 28.34°	96.1 %
Absorption correction	Empirical from SADABS
Max. and min. transmission	0.9137 and 0.7700
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7497 / 0 / 325
Goodness-of-fit on F^2	1.190
Final R indices [I>2sigma(I)]	R1 = 0.0286, wR2 = 0.0690
R indices (all data)	R1 = 0.0396, wR2 = 0.0732
Largest diff. peak and hole	0.470 and -0.597 $e.Å^{-3}$