Data Set 1. Crystal and structure refinement for *Hira08*

Identification Code	Hira08	
Empirical formula	$C_{12}H_{14}BrNO_2$	
Formula weight	284.15	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space Group	$P2_1$	
Unit cell dimensions	a = 10.450(6) Å	α = 90.0°
	b = 8.994(5) Å	β = 101.167(8)°
	c = 13.245(7) Å	γ = 90.0°
Volume	1221.3(11) Å^3	
Z	4	
Density (calculated)	1.545 Mg/m^3	
Absorption coefficient	3.351 mm^{-1}	
F(000)	576	
Crystal size, color, habit	0.40 × 0.25 × 0.05 mm, clear, plate	
Theta range for data collection	1.99 – 25.03°	
Index ranges	$-12 \le h \le 12$, $-10 \le k \le 10$, $-15 \le l \le 15$	
Reflections collected	11,677	
Independent reflections	4,306 (R_{int} = 0.0379)	
Reflections with $I > 4\sigma(F_o)$	3,836	
Flack parameter	0.0212(0.009)	
Absorption correction	SADABS based on redundant diffractions	
Maximum/minimum transmission	1.0/0.594	
Refinement method	Full-matrix least squares on F^2	
Weighting scheme	$w = q\,[\sigma^2 (F_o^2) + (aP)^2 + bP]^{-1}$ where:	
	$P = (F_o^2 + 2F_c^2)/3$, a = 0.0521, b = 0.0, q = 1	
Data/restraints/parameters	4,306/1/289	
Goodness of fit on F^2	0.994	
Final R indices [$I > 2\sigma(I)$]	$R1$ = 0.0380, $wR2$ = 0.0877	
R indices (all data)	$R1$ = 0.0423, $wR2$ = 0.0889	
Largest difference: peak and hole	0.961, –0.294 eÅ^{-3}	