checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: i14503

Bond precision: C-C = 0.0090 A Wavelength=0.71073

Cell: a=26.209•2, b=22.2233•15, c=10.1390•7,
alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	5905.5•7,	5905.5•8,
Space group	A b a 2	A b a 2
Hall group	A 2 -2ac	A 2 -2ac
Moiety formula	C46 H57 B N8, 4•C H2 Cl2,, 2•I,	2•I,, 4•C H2 Cl2,, C46 H57 B N8
Sum formula	C50 H65 B Cl8 I2 N8	C50 H65 B Cl8 I2 N8
Mr	1326.31	1326.38
Dx,g cm-3	1.492	1.492
Z	4	4
Mu •mm-1,	1.467	1.467
F000	2672.0	2674.1
F000'	2673.56	
h,k,lmax	37,31,14	36,30,14
Nref	8755[4609]	7711
Tmin,Tmax	0.900,0.916	0.922,1.000
Tmin'	0.768	

Correction method= MULTI-SCAN

Data completeness= 1.67/0.88 Theta•max,= 30.160

R•reflections,= 0.0597• 5552, wR2•reflections,= 0.1374• 7711,

S = 1.045 Npar= 318

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level .
Click on the hyperlinks for more details of the test.

Alert level C

PLAT068_ALERT_1_C Reported F000 Differs from Calcd •or Missing,... ?
PLAT213_ALERT_2_C Atom C8 has ADP max/min Ratio ..... 3.3 prola
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C24
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C25
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0090 Ang