

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: R-3-Br

Bond precision:	C-C = 0.0237 A	Wavelength=0.71073
Cell:	a=8.795 (2)	b=7.9006 (15) c=18.009 (4)
	alpha=90	beta=97.490 (9) gamma=90
Temperature:	297 K	
	Calculated	Reported
Volume	1240.7 (5)	1240.7 (5)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	Br4 Pb, 2 (C8 H11 Br N)	Br4 Pb, 2 (C8 H11 Br N)
Sum formula	C16 H22 Br6 N2 Pb	C16 H22 Br6 N2 Pb
Mr	928.96	929.00
Dx, g cm ⁻³	2.487	2.487
Z	2	2
Mu (mm ⁻¹)	16.464	16.464
F000	848.0	848.0
F000'	839.11	
h, k, lmax	11, 10, 23	11, 10, 23
Nref	5734 [3076]	5691
Tmin, Tmax	0.523, 0.719	0.223, 0.746
Tmin'	0.512	

Correction method= # Reported T Limits: Tmin=0.223 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.85/0.99 Theta (max)= 27.525

R(reflections)= 0.0410 (4924)	wR2(reflections)= 0.1257 (5691)
S = 1.016	Npar= 230

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 B

PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.02375 Ang.
PLAT987_ALERT_1_B	The Flack x is >> 0 - Do a BASF/TWIN Refinement	Please Check



Alert level C

PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C5 Check
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist. C1 -C6 .	1.37 Ang.
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4	Please Check



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	20 Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6 Report
	H1A H1B H1C H2A H2B H2C	
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero .	0.046 Note
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem C	84 %Fit
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1 Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pb1 --Br1 .	5.9 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pb1 --Br2 .	9.1 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pb1 --Br4 .	8.8 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pb1 --Br1_d .	8.9 s.u.
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb1 (II) .	2.34 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	121 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	8 Note
	0 0 2, -1 1 2, 0 0 10, 0 0 11, 2 0 12, 0 0 13,	
	3 -3 2, 3 3 17,	

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check
-

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

