

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-F

Bond precision:	C-C = 0.0228 A	Wavelength=1.54184
Cell:	a=8.8556(1)	b=7.7361(1) c=16.9816(2)
	alpha=90	beta=96.031(1) gamma=90
Temperature:	200 K	
	Calculated	Reported
Volume	1156.93(2)	1156.93(2)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	Br4 Pb, 2(C8 H11 F N)	Br4 Pb, 2(C8 H11 F N)
Sum formula	C16 H22 Br4 F2 N2 Pb	C16 H22 Br4 F2 N2 Pb
Mr	807.16	807.18
Dx, g cm ⁻³	2.317	2.317
Z	2	2
Mu (mm ⁻¹)	22.438	22.438
F000	744.0	744.0
F000'	731.75	
h,k,lmax	9,8,19	9,8,19
Nref	3418[1855]	3183
Tmin,Tmax	0.469,0.638	0.077,1.000
Tmin'	0.354	

Correction method= # Reported T Limits: Tmin=0.077 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.72/0.93 Theta(max)= 59.993

R(reflections)= 0.0393(3139)	wR2(reflections)= 0.0956(3183)
S = 1.132	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

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5616
PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE. 293 Degree
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds 0.02281 Ang.

Alert level C

PLAT234_ALERT_4_C Large Hirshfeld Difference F1 --C2 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F2 --C10 . 0.18 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C6 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
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pb1 --Br2 . 6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pb1 --Br4 . 6.3 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.41 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 133 Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 120.0 Degree

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

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

