

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20210608\_s4\_d1-2\_autotwinabs\_250k

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: 20210608\_s4\_d1-2\_autotwinabs\_250k

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Bond precision:	N- C = 0.0043 A	Wavelength=0.71073
Cell:	a=9.5183(2)	b=9.5183(2)      c=37.3034(8)
	alpha=90	beta=90      gamma=120
Temperature:	250 K	
	Calculated	Reported
Volume	2926.83(14)	2926.83(14)
Space group	R -3 c	R -3 c
Hall group	-R 3 2" c	-R 3 2" c
Moiety formula	C16 Pb, 2(C3 H10 N), 2(Cl)	C16 Pb1 2-, (C3 H10 N1 1+)2, Cl2
Sum formula	C6 H20 Cl8 N2 Pb	C6 H20 Cl8 N2 Pb
Mr	611.03	611.03
Dx, g cm-3	2.080	2.080
Z	6	6
Mu (mm-1)	9.726	9.726
F000	1728.0	1728.0
F000'	1715.91	
h,k,lmax	14,14,54	0,0,0
Nref	1088	1082
Tmin,Tmax	0.253,0.232	0.080,0.158
Tmin'	0.213	

Correction method= # Reported T Limits: Tmin=0.080 Tmax=0.158  
AbsCorr = MULTI-SCAN

Data completeness= 0.994      Theta(max)= 31.513

R(reflections)= 0.0206( 951)	wR2(reflections)= 0.0401( 1082)
S = 1.112	Npar= 34

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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.

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#### Alert level C

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	10.902	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	4	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF ....	4	Note

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#### Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	1	Report
PLAT019_ALERT_1_G	_diffn_measured_fraction_theta_full/*_max < 1.0	0.998	Report
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ		Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.10	Why ?
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pb1 --Cl1 .	11.3	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl2 Constrained at	0.3333	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 3 )	0.33	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Cl1 ..Cl2 .	2.89	Ang.
	x,y,z =	1_555	Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.11	Ratio
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	1	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb1 (IV) .	4.89	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	1.0	Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....		Please Check

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

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 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  
3 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.

