

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: new

Bond precision:	Pb- O = 0.0127 A	Wavelength=0.71073
Cell:	a=9.8109 (6)	b=9.8109 (6) c=14.8403 (12)
	alpha=90	beta=90 gamma=120
Temperature:	293 K	
	Calculated	Reported
Volume	1237.06 (18)	1237.06 (15)
Space group	P -3	P-3
Hall group	-P 3	?
Moiety formula	O25 P6 Pb10	?
Sum formula	O25 P6 Pb10	O25 P6 Pb10
Mr	2657.82	2657.72
Dx, g cm ⁻³	7.135	7.135
Z	2	2
Mu (mm ⁻¹)	68.270	68.270
F000	2220.0	2220.0
F000'	2162.42	
h, k, lmax	15, 15, 23	15, 15, 23
Nref	3527	3456
Tmin, Tmax	0.023, 0.505	0.339, 1.000
Tmin'	0.012	

Correction method= # Reported T Limits: Tmin=0.339 Tmax=1.000
AbsCorr = ANALYTICAL

Data completeness= 0.980 Theta (max)= 34.530

R(reflections)= 0.0413 (2577)	wR2(reflections)= 0.0771 (3456)
S = 0.866	Npar= 105

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

PLAT112_ALERT_2_B	ADDSYM Detects New (Pseudo) Symm. Elem	61	100 %Fit
PLAT112_ALERT_2_B	ADDSYM Detects New (Pseudo) Symm. Elem	61	100 %Fit



Alert level C

PLAT199_ALERT_1_C	Reported _cell_measurement_temperature	(K)	293	Check
PLAT200_ALERT_1_C	Reported _diffrn_ambient_temperature	(K)	293	Check



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !	
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	3	Units
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	6%	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb1A (II)	.	1.90 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb2A (II)	.	2.05 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb2B (II)	.	2.07 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb2C (II)	.	2.04 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb2D (II)	.	2.05 Info
PLAT899_ALERT_4_G	SHELXL-97 is Deprecated and Succeeded by SHELXL	2019/3	Note

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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
7 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.

