

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) KP2002\_0m\_d

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: KP2002\_0m\_d

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Bond precision:	Pb- O = 0.0060 A	Wavelength=0.71073	
Cell:	a=7.9693 (3)	b=7.9693 (3)	c=9.2741 (3)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	589.00 (5)	589.00 (5)	
Space group	P -4 21 c	P -4 21 c	
Hall group	P -4 2n	P -4 2n	
Moiety formula	H4 O8 Pb6	?	
Sum formula	H4 O8 Pb6	H4 O8 Pb6	
Mr	1375.23	1375.17	
Dx, g cm <sup>-3</sup>	7.754	7.754	
Z	2	2	
Mu (mm <sup>-1</sup> )	85.454	85.455	
F000	1120.0	1120.0	
F000'	1085.63		
h, k, lmax	12, 12, 14	12, 12, 14	
Nref	1302 [ 757]	1304	
Tmin, Tmax	0.373, 0.425	0.414, 0.752	
Tmin'	0.174		

Correction method= # Reported T Limits: Tmin=0.414 Tmax=0.752  
AbsCorr = MULTI-SCAN

Data completeness= 1.72/1.00      Theta(max)= 34.939

R(reflections)= 0.0156 ( 1183)	wR2(reflections)= 0.0320 ( 1304)
S = 1.109	Npar= 35

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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**

PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.57Ang From Pb1	-1.57 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.83Ang From O1	0.83 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	1.08Ang From O1	0.82 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.49Ang From O1	0.65 eA-3

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#### **Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	1 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.52 Why ?
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb1 (II)	1.98 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb2 (II)	1.98 Info
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	70.0 Degree

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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  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
6 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
6 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
0 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.

