

## 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: finescreekite

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Bond precision:    S- O = 0.0500 A                      Wavelength=0.71075

Cell:                      a=8.2330 (9)              b=10.7128 (13)              c=14.8256 (13)  
                                    alpha=90                      beta=90                      gamma=90

Temperature:              293 K

	Calculated	Reported
Volume	1307.6 (2)	1307.6 (2)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	O10 Pb4 S4	?
Sum formula	O10 Pb4 S4	H4 O10 Pb4 S4
Mr	1117.04	1121.03
Dx, g cm <sup>-3</sup>	5.674	5.694
Z	4	4
Mu (mm <sup>-1</sup> )	52.020	52.021
F000	1888.0	1904.0
F000'	1842.57	
h, k, lmax	8, 11, 15	8, 11, 15
Nref	1654 [ 982]	1588
Tmin, Tmax	0.033, 0.353	0.188, 1.000
Tmin'	0.001	

Correction method= # Reported T Limits: Tmin=0.188 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.62/0.96                      Theta (max)= 22.212

R(reflections)= 0.0611 ( 1440)

wR2(reflections)=  
0.1491 ( 1588)

S = 1.062

Npar= 158

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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 A

THETM01\_ALERT\_3\_A The value of sine(theta\_max)/wavelength is less than 0.550  
Calculated sin(theta\_max)/wavelength = 0.5319  
PLAT211\_ALERT\_2\_A ADP of Atom O1 is N.P.D. or (nearly) 2D . Please Check  
PLAT213\_ALERT\_2\_A Atom O6 has ADP max/min Ratio ..... 8.0 prolat

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### Alert level B

RINTA01\_ALERT\_3\_B The value of Rint is greater than 0.18  
Rint given 0.183

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### Alert level C

PLAT029\_ALERT\_3\_C \_diffrn\_measured\_fraction\_theta\_full value Low . 0.968 Why?  
PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
PLAT043\_ALERT\_1\_C Calculated and Reported Mol. Weight Differ by .. 3.99 Check  
PLAT068\_ALERT\_1\_C Reported F000 Differs from Calcd (or Missing)... Please Check  
PLAT090\_ALERT\_3\_C Poor Data / Parameter Ratio (Zmax > 18) ..... 6.22 Note  
PLAT213\_ALERT\_2\_C Atom O2 has ADP max/min Ratio ..... 3.3 prolat  
PLAT213\_ALERT\_2\_C Atom Oh9 has ADP max/min Ratio ..... 3.7 prolat  
PLAT213\_ALERT\_2\_C Atom O5 has ADP max/min Ratio ..... 3.2 prolat  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of O2 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of S1 Check

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### Alert level G

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and the formula from the \_atom\_site\* data.  
Atom count from \_chemical\_formula\_sum: H4 O10 Pb4 S4  
Atom count from the \_atom\_site data: O10 Pb4 S4  
CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
CELLZ01\_ALERT\_1\_G WARNING: H atoms missing from atom site list. Is this intentional?  
From the CIF: \_cell\_formula\_units\_Z 4  
From the CIF: \_chemical\_formula\_sum H4 O10 Pb4 S4  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
H	16.00	0.00	16.00
O	40.00	40.00	0.00
Pb	16.00	16.00	0.00
S	16.00	16.00	0.00

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 3 Info  
PLAT020\_ALERT\_3\_G The Value of Rint is Greater Than 0.12 ..... 0.183 Report  
PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check  
PLAT200\_ALERT\_1\_G Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 4 Note  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 1 Note  
PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 4.7 Low

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

8 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  
6 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
1 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.

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**PLATON version of 19/02/2022; check.def file version of 19/02/2022**

