

## checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . . .

## checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) shelx

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.  
Please wait while processing ....

[CIF dictionary](#)  
[Interpreting this report](#)

[Structure factor report](#)

## Datablock: shelx

Bond precision: P- O = 0.0090 Å Wavelength=0.71073  
 Cell: a=7.2191(10) b=7.2191(10) c=16.834(3)  
 alpha=90 beta=90 gamma=120  
 Temperature: 293 K

	Calculated	Reported
Volume	759.8(3)	759.8(3)
Space group	R -3 m	R -3 m :H
Hall group	-R 3 2"	-R 3 2"
Moiety formula	A13.42 Fe5.58 H18 O42 P6 Pb3	?
Sum formula	A13.42 Fe5.58 H18 O42 P6 Pb3	A13.42 Fe5.58 H18 O42 P6 Pb3
Mr	1901.60	1901.60
Dx, g cm-3	4.156	4.156
Z	1	1
Mu (mm-1)	19.718	19.718
F000	879.6	879.6
F000'	873.10	
h,k,lmax	9,9,21	9,9,21
Nref	243	242
Tmin,Tmax	0.225,0.373	0.426,0.573
Tmin'	0.189	

Correction method= # Reported T Limits: Tmin=0.426 Tmax=0.573 AbsCorr = MULTI-SCAN  
 Data completeness= 0.996 Theta(max)= 27.455  
 R(reflections)= 0.0415( 226) wR2(reflections)= 0.0985( 242)  
 S = 1.228 Npar= 30

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 A

[PLAT430\\_ALERT\\_2\\_A](#) Short Inter D...A Contact O1 ..O2 . 2.50 Ang.  
 $1/3+y, 2/3-x+y, 2/3-z = 32\_555$  Check  
[PLAT430\\_ALERT\\_2\\_A](#) Short Inter D...A Contact O2 ..O2 . 2.48 Ang.  
 $1-x+y, -x, z = 4\_655$  Check  
[PLAT430\\_ALERT\\_2\\_A](#) Short Inter D...A Contact O2 ..O2 . 2.48 Ang.  
 $-y, -1+x-y, z = 2\_545$  Check

### Alert level C

[PLAT077\\_ALERT\\_4\\_C](#) Unitcell Contains Non-integer Number of Atoms .. Please Check  
[PLAT088\\_ALERT\\_3\\_C](#) Poor Data / Parameter Ratio ..... 8.07 Note  
[PLAT313\\_ALERT\\_2\\_C](#) Oxygen with Three Covalent Bonds (rare) ..... O2 Check  
[PLAT975\\_ALERT\\_2\\_C](#) Check Calcd Resid. Dens. 0.99A From O2 0.55 eA-3

**And 2 other PLAT975 Alerts**

More ...

PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.91A From O1 -1.20 eA-3  
 PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.98A From O2 -0.72 eA-3

**Alert level G**

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 2 Note  
 PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 3 Info  
 PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 40.77 Why ?  
 PLAT168\_ALERT\_4\_G The CIF-Embedded .res File Contains EXYZ Records 1 Report  
 PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 1 Report  
 PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 1 Report  
 PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check  
 PLAT200\_ALERT\_1\_G Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check  
 PLAT300\_ALERT\_4\_G Atom Site Occupancy of Pb Constrained at 0.1667 Check  
 PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1 ) 38% Note  
 PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 1 Note  
 PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
 PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note  
 PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 4.8 Low  
 PLAT965\_ALERT\_2\_G The SHELXL WEIGHT Optimisation has not Converged Please Check

3 **ALERT level A** = Most likely a serious problem - resolve or explain  
 0 **ALERT level B** = A potentially serious problem, consider carefully  
 8 **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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 12 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  
 1 ALERT type 5 Informative message, check

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.

PLATON version of 13/07/2021; check.def file version of 13/07/2021

**Datablock shelx - ellipsoid plot**

