

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 _diffn_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

