

## checkCIF/PLATON report

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.      CIF dictionary      Interpreting this report

### Datablock: shelx

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Bond precision:	= 0.0000 A	Wavelength=0.71073
Cell:	a=10.4365 (5)	b=10.4365 (5)      c=10.4365 (5)
	alpha=90	beta=90      gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	1136.75 (16)	1136.75 (17)
Space group	I -4 3 m	I -4 3 m
Hall group	I -4 2 3	I -4 2 3
Moiety formula	Ag <sub>6.36</sub> As <sub>4.24</sub> Cu <sub>13.64</sub> Fe <sub>4</sub> S <sub>26</sub> Sb <sub>3.76</sub>	?
Sum formula	Ag <sub>6.36</sub> As <sub>4.24</sub> Cu <sub>13.64</sub> Fe <sub>4</sub> S <sub>26</sub> Sb <sub>3.76</sub>	Ag <sub>3.18</sub> As <sub>2.12</sub> Cu <sub>6.82</sub> Fe <sub>2</sub> S <sub>13</sub> Sb <sub>1.88</sub>
Mr	3385.32	1692.66
Dx, g cm <sup>-3</sup>	4.945	4.945
Z	1	2
Mu (mm <sup>-1</sup> )	16.579	16.579
F000	1546.2	1546.2
F000'	1547.79	
h, k, lmax	13, 13, 13	13, 13, 13
Nref	284 [ 164]	284
Tmin, Tmax	0.565, 0.661	0.076, 0.136
Tmin'	0.554	

Correction method= # Reported T Limits: Tmin=0.076 Tmax=0.136

AbsCorr = MULTI-SCAN

Data completeness= 1.73/1.00

Theta(max)= 28.152

R(reflections)= 0.0384( 246)

wR2(reflections)=  
0.0984( 284)

S = 1.162

Npar= 20

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

PLAT220\_ALERT\_2\_B NonSolvent Resd 1 S Ueq(max)/Ueq(min) Range 7.6 Ratio



#### Alert level C

PLAT077\_ALERT\_4\_C Unitcell Contains Non-integer Number of Atoms .. Please Check  
PLAT220\_ALERT\_2\_C NonSolvent Resd 1 Cu Ueq(max)/Ueq(min) Range 3.6 Ratio  
PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.37Ang From M2AG 1.79 eA-3  
PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 1.03Ang From M2CU 1.70 eA-3



#### Alert level G

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 3 Info  
PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 0.500 Check  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 31.56 Why ?  
PLAT168\_ALERT\_4\_G The CIF-Embedded .res File Contains EXYZ Records 3 Report  
PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 3 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 M1CU Constrained at 0.6667 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of M1FE Constrained at 0.3333 Check  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1) 76% Note  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 6 Note  
M2AG M2CU M1CU M1FE X3AS X3SB  
PLAT811\_ALERT\_5\_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT899\_ALERT\_4\_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note  
PLAT965\_ALERT\_2\_G The SHELXL WEIGHT Optimisation has not Converged Please Check  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 1.77 Note  
Predicted wR2: Based on SigI\*\*2 5.56 or SHELX Weight 8.79

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

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

