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

```
Bond precision:   = 0.0000 A                Wavelength=0.71073

Cell:              a=10.8601(3)      b=10.8601(3)      c=10.8601(3)
                   alpha=90          beta=90           gamma=90
Temperature:       293 K
```

	Calculated	Reported
Volume	1280.86(11)	1280.86(11)
Space group	I -4 3 m	I -4 3 m
Hall group	I -4 2 3	I -4 2 3
Moiety formula	Ag20.75 As7.16 Fe3.24 S26 Sb0.84	?
Sum formula	Ag20.75 As7.16 Fe3.24 S26 Sb0.84	Ag10.37 As3.58 Fe1.62 S13 Sb0.42
Mr	3891.31	1945.66
Dx,g cm-3	5.045	5.045
Z	1	2
Mu (mm-1)	14.702	14.702
F000	1754.5	1754.5
F000'	1740.52	
h,k,lmax	16,16,16	16,16,16
Nref	438[249]	438
Tmin,Tmax	0.499,0.643	0.915,0.946
Tmin'	0.475	

```
Correction method= # Reported T Limits: Tmin=0.915 Tmax=0.946
AbsCorr = MULTI-SCAN

Data completeness= 1.76/1.00        Theta(max)= 31.708
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R(reflections)= 0.0551(400)

wR2(reflections)= 0.1616(438)

S = 1.160 Npar= 22

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 C

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.55Ang From M2B 1.97 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.58Ang From M2B 1.81 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2A as AG
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2B as AG
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 18.28 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 2 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 X3SB Constrained at 0.105 Check
PLAT300_ALERT_4_G Atom Site Occupancy of X3AS Constrained at 0.895 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 78% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 6 Note
M2A M2B M1AG M1FE X3AS X3SB
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 with s.u. 0.11 Check
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 ..... 6.20 Note
Predicted wR2: Based on SigI**2 2.61 or SHELX Weight 14.30

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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
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
19 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
8 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.

PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock shelx - ellipsoid plot