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=10.6580(19)     b=10.6580(19)     c=10.6580(19)
                  alpha=90          beta=90           gamma=90
Temperature:      293 K
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	Calculated	Reported
Volume	1210.7(6)	1210.7(6)
Space group	I -4 3 m	I -4 3 m
Hall group	I -4 2 3	I -4 2 3
Moiety formula	Cu4 S1.13 Se6.87, 0.04(Cu24), 1.637(Te), 0.207(Se), 1.029(As),	?
Sum formula	As1.03 Cu8 S1.59 Se7.08 Te1.64	As1.545 Cu12 S2.385 Se10.615 Te2.455
Mr	1404.28	2106.42
Dx,g cm-3	5.778	5.778
Z	3	2
Mu (mm-1)	31.458	31.458
F000	1851.6	1851.6
F000'	1857.10	
h,k,lmax	16,16,16	13,14,13
Nref	464[263]	410
Tmin,Tmax	0.475,0.533	0.475,0.533
Tmin'	0.451	

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Correction method= # Reported T Limits: Tmin=0.475 Tmax=0.533
AbsCorr = MULTI-SCAN

Data completeness= 1.56/0.88        Theta(max)= 33.221
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R(reflections)= 0.0285(334)

wR2(reflections)= 0.0512(410)

S = 1.070 Npar= 24

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

PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ	Please Check	
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check	
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.00Ang From Se2	1.92	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 2.26Ang From Se1	1.55	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	CU	
PLAT017_ALERT_1_G	Check Scattering Type Consistency of M2B as	CU	
PLAT017_ALERT_1_G	Check Scattering Type Consistency of M1 as	CU	
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	1.500	Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
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	4	Report
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3	Note
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1)	62%	Note
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 7)	100%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact Te ..Se1 .	2.48	Ang.
	x,y,z = 1_555	Check	
PLAT432_ALERT_2_G	Short Inter X...Y Contact Te ..Se1 .	2.48	Ang.
	y,z,x = 9_555	Check	
PLAT432_ALERT_2_G	Short Inter X...Y Contact Te ..Se1 .	2.48	Ang.
	z,x,y = 17_555	Check	
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	3	Note
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
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	11	Note
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	3	Units
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2	Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	3	Units
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by .	1	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.	2	Units
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check	

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

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  0 ALERT level B = A potentially serious problem, consider carefully
  4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 32 ALERT level G = General information/check it is not something unexpected

 11 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
  2 ALERT type 3 Indicator that the structure quality may be low
 12 ALERT type 4 Improvement, methodology, query or suggestion
  5 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.

PLATON version of 06/07/2023; check.def file version of 30/06/2023

Datablock shelx - ellipsoid plot