

## 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=3.633 (7)	b=3.633 (7)	c=6.365 (12)
	alpha=90	beta=90	gamma=120
Temperature:	293 K		
	Calculated	Reported	
Volume	72.8 (3)	72.7 (3)	
Space group	P -3 m 1	P -3 m 1	
Hall group	-P 3 2"	-P 3 2"	
Moiety formula	Se0.42 Te1.58 V, 0.099 (V)	?	
Sum formula	Se0.42 Te1.58 V1.10	Se0.42 Te1.58 V1.10	
Mr	290.75	290.81	
Dx, g cm <sup>-3</sup>	6.630	6.639	
Z	1	1	
Mu (mm <sup>-1</sup> )	24.116	24.140	
F000	121.7	122.0	
F000'	121.23		
h, k, lmax	5, 5, 9	5, 5, 9	
Nref	113	111	
Tmin, Tmax	0.158, 0.185	0.383, 0.746	
Tmin'	0.133		

Correction method= # Reported T Limits: Tmin=0.383 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.982      Theta(max)= 31.001

R(reflections)= 0.0192 ( 107)	wR2(reflections)= 0.0416 ( 111)
S = 0.987	Npar= 14

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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.

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#### Alert level B

PLAT088\_ALERT\_3\_B Poor Data / Parameter Ratio ..... 7.93 Note

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#### Alert level C

PLAT077\_ALERT\_4\_C Unitcell Contains Non-integer Number of Atoms .. Please Check  
PLAT148\_ALERT\_3\_C s.u. on the a - Axis is (Too) Large .... 0.007 Ang.  
PLAT148\_ALERT\_3\_C s.u. on the c - Axis is (Too) Large .... 0.012 Ang.  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of V1 Check

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#### Alert level G

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 2 Info  
PLAT068\_ALERT\_1\_G Reported F000 Differs from Calcd (or Missing)... Please Check  
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 ) 88% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 100% 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 1 Note  
PLAT961\_ALERT\_5\_G Dataset Contains no Negative Intensities ..... Please Check  
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  
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  
12 **ALERT level G** = General information/check it is not something unexpected

- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 ALERT type 2 Indicator that the structure model may be wrong or deficient  
4 ALERT type 3 Indicator that the structure quality may be low  
4 ALERT type 4 Improvement, methodology, query or suggestion  
3 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.

