

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:	C-C = 0.0020 A	Wavelength=0.71073	
Cell:	a=5.25999(11)	b=12.9652(4)	c=16.6417(4)
	alpha=90	beta=90	gamma=90
Temperature:	123 K		
	Calculated	Reported	
Volume	1134.91(5)	1134.91(5)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C18 H11.96 Te0.02	C18 H11.96 Te0.02	
Sum formula	C18 H11.96 Te0.02	C18 H11.96 Te0.02	
Mr	230.79	230.79	
Dx,g cm-3	1.351	1.351	
Z	4	4	
Mu (mm-1)	0.126	0.126	
F000	484.0	484.0	
F000'	484.14		
h,k,lmax	9,23,30	9,23,30	
Nref	7466[4211]	7319	
Tmin,Tmax	0.966,0.984	0.898,0.962	
Tmin'	0.939		

Correction method= ANALYTICAL

Data completeness= 1.74/0.98 Theta(max)= 40.978

R(reflections)= 0.0639(5466) wR2(reflections)= 0.1641(7319)

S = 1.066 Npar= Npar = 174

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
PLAT234_ALERT_4_C	Large Hirshfeld Difference Tel -- C7 ..	0.17 Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	4.197 Check
PLAT910_ALERT_3_C	Missing # of FCF Reflections Below Th(Min)	5 Why ?
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	9 Why ?

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3 Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Dimension	1 Info
PLAT230_ALERT_2_G	Hirshfeld Test Diff for Tel -- C18 ..	7.3 su
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage = 0 Note
PLAT333_ALERT_2_G	Check Large Av C6-Ring C-C Dist. C1 -C6	1.44 Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	2 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	47 Note

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 3 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
 - 3 ALERT type 4 Improvement, methodology, query or suggestion
 - 1 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*, 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 05/02/2014; check.def file version of 05/02/2014

Datablock shelx - ellipsoid plot

