

# 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 = 0.0045 A                      Wavelength=1.54184

Cell:                      a=5.2728(3)              b=13.3470(11)              c=16.7410(11)  
                                    alpha=90                      beta=90                      gamma=90  
Temperature:              123 K

	Calculated	Reported
Volume	1178.17(14)	1178.17(14)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C18 H11.19 Se0.40	C18 H11.19 Se0.40
Sum formula	C18 H11.19 Se0.40	C18 H11.19 Se0.40
Mr	259.36	259.44
Dx,g cm-3	1.462	1.463
Z	4	4
Mu (mm-1)	1.992	1.996
F000	531.7	532.0
F000'	531.66	
h,k,lmax	6,16,20	6,16,20
Nref	2373[ 1407]	1899
Tmin,Tmax	0.727,0.823	0.560,0.828
Tmin'	0.366	

Correction method= ANALYTICAL

Data completeness= 1.35/0.80                      Theta(max)= 73.300

R(reflections)= 0.0389( 1797)                      wR2(reflections)= 0.1133( 1899)

S = 1.077                                              Npar= Npar = 183

---

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

PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT077_ALERT_4_C	Unitcell contains non-integer number of atoms ..	Please Check
PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18) .....	7.47 Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....	2.1 Note
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	3 Why ?
PLAT915_ALERT_3_C	Low Friedel Pair Coverage .....	55 %

### ● Alert level G

PLAT301_ALERT_3_G	Main Residue Disorder .....	Percentage =	24 Note
PLAT333_ALERT_2_G	Check Large Av C6-Ring C-C Dist. C1 -C6		1.44 Ang.
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....		! Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		37 Note

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

