

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 = 0.0092 A Wavelength=1.54178

Cell: a=5.2507(5) b=13.804(2) c=16.782(2)
 alpha=90 beta=90 gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	1216.4(3)	1216.4(3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C18 H11.27 Se0.36	C18 H11.27 Se0.36
Sum formula	C18 H11.27 Se0.36	C18 H11.27 Se0.36
Mr	256.21	256.17
Dx,g cm-3	1.399	1.399
Z	4	4
Mu (mm-1)	1.788	1.786
F000	526.5	526.0
F000'	526.54	
h,k,lmax	6,17,21	6,17,21
Nref	2548[1507]	2489
Tmin,Tmax	0.761,0.898	0.702,1.000
Tmin'	0.397	

Correction method= MULTI-SCAN

Data completeness= 1.65/0.98 Theta(max)= 76.148

R(reflections)= 0.0805(1702) wR2(reflections)= 0.2802(2489)

S = 1.065 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

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
Weighted R factor given 0.280

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
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.28	Why ?
PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	8.13	Note
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.68	Why ?
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0092	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H2A .. SE1 ..	3.00	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H2A .. SE2 ..	3.08	Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. # C18 H11.27 Se0.36		1 Note
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	3.584	Check

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		3 Why ?
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.	0.18	Why ?
PLAT301_ALERT_3_G	Main Residue Disorder	24	Note
PLAT333_ALERT_2_G	Check Large Av C6-Ring C-C Dist. C5 -C18	1.43	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	3	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	18	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflections Below Th(Min)	1	Why ?
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		20 Note

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

0 **ALERT level B** = A potentially serious problem, consider carefully

11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

9 **ALERT level G** = General information/check it is not something unexpected

1 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

8 ALERT type 3 Indicator that the structure quality may be low

6 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

