

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cf1707

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: cf1707

Bond precision:	C-C = 0.0041 A	Wavelength=0.71075
Cell:	a=9.3421(10)	b=19.570(2) c=23.901(3)
	alpha=90	beta=90.387(3) gamma=90
Temperature:	123 K	
	Calculated	Reported
Volume	4369.6(8)	4369.6(8)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C47 H69 Cl Ge N2 S	C47 H69 Cl Ge N2 S
Sum formula	C47 H69 Cl Ge N2 S	C47 H69 Cl Ge N2 S
Mr	802.16	802.14
Dx,g cm-3	1.219	1.219
Z	4	4
Mu (mm-1)	0.843	0.843
F000	1720.0	1720.0
F000'	1722.11	
h,k,lmax	12,25,31	12,25,31
Nref	10001	9966
Tmin,Tmax	0.951,0.983	0.939,0.980
Tmin'	0.919	

Correction method= # Reported T Limits: Tmin=0.939 Tmax=0.980
AbsCorr = NUMERICAL

Data completeness= 0.997 Theta(max)= 27.484

R(reflections)= 0.0486(6471) wR2(reflections)= 0.1243(9966)

S = 0.906 Npar= 487

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 B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 14 Note

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as Numerical

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.136

PLAT412_ALERT_2_C Short Intra XH3 .. XHn H109 ..H116 1.88 Ang.

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 18 Report

Alert level G

PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 0.136 Report

PLAT898_ALERT_4_G Second Reported H-M Symbol in CIF Ignored ! Check

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 3 Note

PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 16 Note

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

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

- 1 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
4 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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* 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.

