

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo\_b3416\_0m

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: mo\_b3416\_0m

---

Bond precision:	C-C = 0.0021 Å	Wavelength=0.71073
Cell:	a=10.8275(14) alpha=90	b=5.6092(8) beta=94.473(5) c=27.626(3) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	1672.7(4)	1672.7(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C10 H13 N O S, C6 H8 N, Cl	Cl, C10 H13 N O S, C6 H8 N
Sum formula	C16 H21 Cl N2 O S	C16 H21 Cl N2 O S
Mr	324.86	324.86
Dx, g cm <sup>-3</sup>	1.290	1.290
Z	4	4
Mu (mm <sup>-1</sup> )	0.354	0.354
F000	688.0	688.0
F000'	689.30	
h,k,lmax	13,7,34	13,7,34
Nref	3416	3412
Tmin,Tmax	0.905,0.968	0.396,0.562
Tmin'	0.769	

Correction method= # Reported T Limits: Tmin=0.396 Tmax=0.562  
AbsCorr = MULTI-SCAN

Data completeness= 0.999      Theta(max)= 26.400

R(reflections)= 0.0349( 2973)	wR2(reflections)= 0.0899( 3412)
S = 1.059	Npar= 192

---

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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
	Calc: C10 H13 N O S, C6 H8 N, Cl	
	Rep.: Cl, C10 H13 N O S, C6 H8 N	
PLAT230_ALERT_2_C	Hirshfeld Test Diff for S1 --C1 .	5.1 s.u.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.735 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2 Report
	-5 0 3, -4 0 4,	

---



### Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	4 Report
	H1 H2A H2B H2C	
PLAT063_ALERT_4_G	Crystal Size Possibly too Large for Beam Size ..	0.74 mm
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3 Note
	Cl	
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2 Note
	-1 0 1, 0 0 2,	
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3 Note
	-5 0 3, -4 0 4, -1 0 1,	
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....	2.834 Note
	Predicted wR2: Based on SigI**2 3.17 or SHELX Weight 8.49	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	15 Info

---

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
8 **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  
3 ALERT type 3 Indicator that the structure quality may be low  
3 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

