**checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) 830\_0m\_a

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](http://journals.iucr.org/services/cif/checking/checkcifreport.html)

**Datablock: 830\_0m\_a**

Bond precision: C-C = 0.0062 A Wavelength=0.71073

|  |  |  |  |
| --- | --- | --- | --- |
| Cell: | a=12.468(4) | b=10.781(3) | c=17.754(4) |
|  | alpha=90 | beta=108.048(12) | gamma=90 |
| Temperature: | 293 K |  |  |

Calculated Reported Volume 2269.0(11) 2268.9(10) Space group P 21/n P 1 21/n 1

Hall group -P 2yn -P 2yn

Moiety formula C22 H16 Cl2 F3 O4 Sb C22 H16 Cl2 F3 O4 Sb Sum formula C22 H16 Cl2 F3 O4 Sb C22 H16 Cl2 F3 O4 Sb Mr 594.01 594.00

Dx,g cm-3 1.739 1.739

Z 4 4

Mu (mm-1) 1.503 1.503

F000 1168.0 1168.0

F000’ 1167.44

h,k,lmax 21,18,31 21,18,31

Nref 12950 12882

Tmin,Tmax 0.365,0.582 0.561,0.748

Tmin’ 0.316

Correction method= # Reported T Limits: Tmin=0.561 Tmax=0.748

AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 38.730

R(reflections)= 0.0532( 8317) wR2(reflections)= 0.1327( 12882) S = 1.089 Npar= 289

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**

PLAT241\_ALERT\_2\_C High ’MainMol’ Ueq as Compared to Neighbors of C25 Check PLAT242\_ALERT\_2\_C Low ’MainMol’ Ueq as Compared to Neighbors of C14 Check PLAT242\_ALERT\_2\_C Low ’MainMol’ Ueq as Compared to Neighbors of C24 Check PLAT334\_ALERT\_2\_C Small Aver. Benzene C-C Dist C1 -C6 1.37 Ang. PLAT334\_ALERT\_2\_C Small Aver. Benzene C-C Dist C21 -C26 1.37 Ang. PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ...... 2.379 Check PLAT910\_ALERT\_3\_C Missing # of FCF Reflection(s) Below Theta(Min). 6 Note PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 2.13A From O1 1.71 eA-3

PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 1.05A From O1 0.44 eA-3

**Alert level G**

PLAT005\_ALERT\_5\_G No Embedded Refinement Details Found in the CIF Please Do ! PLAT063\_ALERT\_4\_G Crystal Size Likely too Large for Beam Size .... 0.74 mm PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check PLAT200\_ALERT\_1\_G Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 11 Do !

O2 -SB1 -O1 -C7 -174.00 2.00 1.555 1.555 1.555 1.555

PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 21 Do !

O1 -SB1 -O2 -C9 176.00 16.00 1.555 1.555 1.555 1.555

PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 61 Note

PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 4 Info

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

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

9 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

8 ALERT type 2 Indicator that the structure model may be wrong or deficient

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

4 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* or *IUCrData*[, you should make sure that full publication checks](http://journals.iucr.org/services/cif/checking/checkform.html) 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 07/08/2019; check.def file version of 30/07/2019**

**Datablock 830\_0m\_a** - ellipsoid plot

