**checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) 1080\_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: 1080\_0m\_a**

Bond precision: C-C = 0.0095 A Wavelength=0.71073

|  |  |  |  |
| --- | --- | --- | --- |
| Cell: | a=11.684(11) | b=12.639(11) | c=13.052(14) |
|  | alpha=61.88(3) | beta=63.33(4) | gamma=80.80(3) |
| Temperature: | 293 K |  |  |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Calculated |  |  | Reported |
| Volume | 1516(3) |  |  | 1516(2) |
| Space group | P -1 |  |  | P -1 |
| Hall group | -P 1 |  |  | -P 1 |
| Moiety formula | C26 H12 F17 | O4 | Sb | C26 H12 F17 O4 Sb |
| Sum formula | C26 H12 F17 | O4 | Sb | C26 H12 F17 O4 Sb |
| Mr | 833.12 |  |  | 833.11 |
| Dx,g cm-3 | 1.825 |  |  | 1.825 |
| Z | 2 |  |  | 2 |
| Mu (mm-1) | 1.046 |  |  | 1.047 |
| F000 | 808.0 |  |  | 808.0 |
| F000’ | 807.60 |  |  |  |
| h,k,lmax | 17,19,19 |  |  | 17,19,19 |
| Nref | 11358 |  |  | 11054 |
| Tmin,Tmax | 0.441,0.551 |  |  | 0.453,0.587 |
| Tmin’ | 0.386 |  |  |  |

Correction method= # Reported T Limits: Tmin=0.453 Tmax=0.587

AbsCorr = MULTI-SCAN

Data completeness= 0.973 Theta(max)= 32.940

R(reflections)= 0.0559( 8160) wR2(reflections)= 0.1743( 11054) S = 1.063 Npar= 434

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**

[PLAT230\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT230.html) Hirshfeld Test Diff for F14 --C37 . 12.0 s.u. [PLAT234\_ALERT\_4\_B](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference F15 --C38 . 0.27 Ang. [PLAT242\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C33 Check

**Alert level C**

[ABSTY02\_ALERT\_1\_C](http://journals.iucr.org/services/cif/checking/ABSTY_02.html) 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 multi-scan

[PLAT029\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT029.html) \_diffrn\_measured\_fraction\_theta\_full value Low . 0.973 Why? [PLAT031\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT031.html) Refined Extinction Parameter Within Range ...... 3.000 Sigma [PLAT148\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT148.html) s.u. on the c - Axis is (Too) Large .... 0.014 Ang. [PLAT155\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT155.html) The Triclinic Unitcell is NOT Reduced .......... Please Do ! [PLAT220\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT220.html) Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio [PLAT220\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT220.html) Non-Solvent Resd 1 F Ueq(max)/Ueq(min) Range 3.6 Ratio [PLAT230\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT230.html) Hirshfeld Test Diff for F9 --C34 . 6.8 s.u. [PLAT230\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT230.html) Hirshfeld Test Diff for O3 --C35 . 6.5 s.u. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference F13 --C37 . 0.19 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference F16 --C38 . 0.22 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference F17 --C38 . 0.18 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C37 --C38 . 0.17 Ang. [PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C4 Check [PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C14 Check [PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C32 Check [PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C35 Check [PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C36 Check [PLAT260\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT260.html) Large Average Ueq of Residue Including Sb1 0.121 Check [PLAT342\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT342.html) Low Bond Precision on C-C Bonds ............... 0.0095 Ang. [PLAT910\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT910.html) Missing # of FCF Reflection(s) Below Theta(Min). 8 Note [PLAT911\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT911.html) Missing FCF Refl Between Thmin & STh/L= 0.600 6 Report [PLAT973\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT973.html) Check Calcd Positive Resid. Density on Sb1 1.07 eA-3

[PLAT978\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT978.html) Number C-C Bonds with Positive Residual Density. 0 Info

|  |  |  |
| --- | --- | --- |
|  **Alert level** | **G** |  |
| [PLAT012\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT012.html) | No | \_shelx\_res\_checksum Found in CIF ...... | Please | Check |

[PLAT063\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT063.html) Crystal Size Likely too Large for Beam Size .... 0.90 mm

[PLAT199\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT199.html) Reported \_cell\_measurement\_temperature ..... (K) 293 Check [PLAT200\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT200.html) Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check [PLAT242\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C34 Check [PLAT242\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C38 Check [PLAT710\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT710.html) Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 11 Do !

O1 -SB1 -O3 -C35 -117.00 13.00 1.555 1.555 1.555 1.555

[PLAT710\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT710.html) Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 21 Do !

O3 -SB1 -O1 -C31 1.00 14.00 1.555 1.555 1.555 1.555

[PLAT912\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT912.html) Missing # of FCF Reflections Above STh/L= 0.600 293 Note [PLAT933\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT933.html) Number of OMIT Records in Embedded .res File ... 6 Note [PLAT992\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT992.html) Repd & Actual \_reflns\_number\_gt Values Differ by 2 Check

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

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

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

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

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

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

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

11 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 1080\_0m\_a- ellipsoid plot**

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