**checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) 1915\_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: 1915\_0m\_a**

Bond precision: C-C = 0.0145 A Wavelength=0.71073

|  |  |  |  |
| --- | --- | --- | --- |
| Cell: | a=13.776(11) | b=20.592(19) | c=12.408(13) |
|  | alpha=90 | beta=121.73(4) | gamma=90 |
| Temperature: | 293 K |  |  |

Calculated Reported Volume 2994(5) 2994(5) Space group C 2/c C 1 2/c 1

Hall group -C 2yc -C 2yc

Moiety formula C36 H25 Bi O4 C36 H25 Bi O4

Sum formula C36 H25 Bi O4 C36 H25 Bi O4

Mr 730.54 730.54

Dx,g cm-3 1.621 1.621

Z 4 4

Mu (mm-1) 5.926 5.927

F000 1424.0 1424.0

F000’ 1408.51

h,k,lmax 18,27,16 18,27,16

Nref 3585 3569

Tmin,Tmax 0.030,0.888 0.297,0.746

Tmin’ 0.015

Correction method= # Reported T Limits: Tmin=0.297 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 27.890

R(reflections)= 0.0433( 3332) wR2(reflections)= 0.1267( 3569) S = 1.068 Npar= 187

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**

PLAT148\_ALERT\_3\_C s.u. on the c - Axis is (Too) Large .... 0.013 Ang. PLAT241\_ALERT\_2\_C High ’MainMol’ Ueq as Compared to Neighbors of C13 Check PLAT242\_ALERT\_2\_C Low ’MainMol’ Ueq as Compared to Neighbors of C11 Check PLAT342\_ALERT\_3\_C Low Bond Precision on C-C Bonds ............... 0.01447 Ang. PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.87A From Bi1 -2.14 eA-3

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 1.05A From Bi1 -1.76 eA-3

PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.75A From O1 0.52 eA-3

PLAT977\_ALERT\_2\_C Check Negative Difference Density on H14 -0.41 eA-3

**Alert level G**

PLAT012\_ALERT\_1\_G No \_shelx\_res\_checksum Found in CIF ...... Please Check PLAT063\_ALERT\_4\_G Crystal Size Possibly too Large for Beam Size .. 0.65 mm PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 29.41 Why ? PLAT128\_ALERT\_4\_G Alternate Setting for Input Space Group C2/c I2/a Note PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check PLAT200\_ALERT\_1\_G Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check PLAT371\_ALERT\_2\_G Long C(sp2)-C(sp1) Bond C21 - C27 . 1.45 Ang. PLAT371\_ALERT\_2\_G Long C(sp2)-C(sp1) Bond C28 - C29 . 1.46 Ang. PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 6 Do !

O1 -BI1 -O1 -C29 -179.00 0.50 2.555 1.555 1.555 1.555

PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 15 Do !

O1 -C29 -C28 -C27 84.00 13.00 1.555 1.555 1.555 1.555

PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 16 Do !

O2 -C29 -C28 -C27 -96.00 13.00 1.555 1.555 1.555 1.555

PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 30 Do !

C29 -C28 -C27 -C21 7.00 26.00 1.555 1.555 1.555 1.555

PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 31 Do !

C28 -C27 -C21 -C26 -74.00 15.00 1.555 1.555 1.555 1.555

PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 32 Do !

C28 -C27 -C21 -C22 104.00 15.00 1.555 1.555 1.555 1.555

PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 4 Note PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 13 Note PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ........... 1.0 Low PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 0 Info

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

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

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

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

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

10 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

9 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](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 18/09/2020; check.def file version of 20/08/2020**

**Datablock 1915\_0m\_a- ellipsoid plot**

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lf)

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N

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ro

NOMOVE FORCED Prob

Temp

cs ?

C6 :ml·Q7C5 a

Cl\_a llC4\_a

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lf)

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R 0.04

RES= 0 0 X