**checkCIF/PLATON report**

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 1934\_0m\_a**

Bond precision: C-C = 0.0098 A Wavelength=0.71073

|  |  |  |  |
| --- | --- | --- | --- |
| Cell: | a=12.456(8) | b=12.713(9) | c=13.357(9) |
|  | alpha=86.23(3) | beta=71.82(3) | gamma=69.78(2) |
| Temperature: | 293 K |  |  |

Calculated Reported Volume 1884(2) 1884(2) Space group P -1 P -1

Hall group -P 1 -P 1

Moiety formula C32 H21 Bi N4 O12, C6 H6 C32 H21 Bi N4 O12, 1(C6

H6)

Sum formula C38 H27 Bi N4 O12 C38 H27 Bi N4 O12

Mr 940.62 940.61

|  |  |  |
| --- | --- | --- |
| Dx,g cm-3 | 1.658 | 1.659 |
| Z | 2 | 2 |
| Mu (mm-1) | 4.748 | 4.749 |
| F000 | 924.0 | 924.0 |
| F000’ | 916.36 |  |
| h,k,lmax | 15,15,16 | 14,15,16 |
| Nref | 6918 | 6845 |
| Tmin,Tmax | 0.510,0.593 | 0.576,0.745 |
| Tmin’ | 0.238 |  |

Correction method= # Reported T Limits: Tmin=0.576 Tmax=0.745

AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 25.390

R(reflections)= 0.0373( 5297) wR2(reflections)= 0.0874( 6845) S = 1.050 Npar= 479

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**

[PLAT094\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT094.html) Ratio of Maximum / Minimum Residual Density .... 3.14 Report [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C13 --C14 . 0.16 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C15 --C16 . 0.16 Ang. [PLAT241\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT241.html) High ’MainMol’ Ueq as Compared to Neighbors of O2 Check [PLAT241\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT241.html) High ’MainMol’ Ueq as Compared to Neighbors of C23 Check [PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of N1 Check [PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of N2 Check [PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of N3 Check [PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C21 Check [PLAT250\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT250.html) Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.4 Note [PLAT250\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT250.html) Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.4 Note [PLAT260\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT260.html) Large Average Ueq of Residue Including C51B 0.102 Check [PLAT260\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT260.html) Large Average Ueq of Residue Including C51A 0.102 Check [PLAT331\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT331.html) Small Aver Phenyl C-C Dist C11 --C16 . 1.36 Ang. [PLAT334\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT334.html) Small Aver. Benzene C-C Dist C31 -C36 1.37 Ang. [PLAT342\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT342.html) Low Bond Precision on C-C Bonds ............... 0.00984 Ang.

**Alert level G**

[PLAT003\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT003.html) Number of Uiso or Uij Restrained non-H Atoms ... 6 Report [PLAT042\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT042.html) Calc. and Reported Moiety Formula Strings Differ Please Check [PLAT171\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT171.html) The CIF-Embedded .res File Contains EADP Records 6 Report [PLAT178\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT178.html) The CIF-Embedded .res File Contains SIMU Records 1 Report [PLAT186\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT186.html) The CIF-Embedded .res File Contains ISOR Records 1 Report [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 [PLAT302\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT302.html) Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 100% Note [PLAT302\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT302.html) Anion/Solvent/Minor-Residue Disorder (Resd 3 ) 100% Note [PLAT304\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT304.html) Non-Integer Number of Atoms in ..... (Resd 2 ) 6.29 Check [PLAT304\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT304.html) Non-Integer Number of Atoms in ..... (Resd 3 ) 5.71 Check [PLAT860\_ALERT\_3\_G](http://journals.iucr.org/services/cif/checking/PLAT860.html) Number of Least-Squares Restraints ............. 72 Note [PLAT883\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT883.html) No Info/Value for \_atom\_sites\_solution\_primary . Please Do ! [PLAT933\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT933.html) Number of OMIT Records in Embedded .res File ... 4 Note

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

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

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

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

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

15 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

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 22/03/2021; check.def file version of 19/03/2021**

**Datablock 1934\_0m\_a- ellipsoid plot**

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