

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

---

Bond precision:    C-C = 0.1100 Å                      Wavelength=0.71073

Cell:                      a=12.0170(5)              b=15.3261(6)              c=7.8100(3)  
                                alpha=90                      beta=90                      gamma=90

Temperature:              138 K

	Calculated	Reported
Volume	1438.40(10)	1438.40(10)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	Bi I4, C5 H5 N3	C5 H7 Bi I4 N3
Sum formula	C5 H5 Bi I4 N3	C5 H7 Bi I4 N3
Mr	823.70	825.72
Dx,g cm-3	3.804	3.813
Z	4	4
Mu (mm-1)	20.812	20.812
F000	1404.0	1412.0
F000'	1381.65	
h,k,lmax	14,18,9	14,18,9
Nref	1416	1412
Tmin,Tmax	0.055,0.101	
Tmin'	0.035	

Correction method= Not given

Data completeness= 0.997                      Theta(max)= 25.988

R(reflections)= 0.1333( 1411)              wR2(reflections)= 0.3389( 1412)

S = 1.033                      Npar= 67

---

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 A

DIFF003\_ALERT\_1\_A \_diffrn\_measurement\_device\_type is missing

Diffractometer make and type. Replaces \_diffrn\_measurement\_type.

PLAT058_ALERT_1_A	Maximum Transmission Factor Missing .....	?
PLAT059_ALERT_1_A	Minimum Transmission Factor Missing .....	?
PLAT342_ALERT_3_A	Low Bond Precision on C-C Bonds .....	0.11 Ang.
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 0.95A From I1	7.45 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.56A From C2	5.94 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 2.00A From C4	5.90 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.11A From N3	5.82 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 0.78A From I2	5.76 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.76A From N1	5.61 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 0.70A From I1	4.84 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.57A From C1	4.81 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.62A From I2	4.78 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 2.41A From I1	4.72 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 0.69A From I1	4.69 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.85A From N3	4.64 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.66A From I1	4.57 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.68A From I2	4.38 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 2.14A From N3	4.30 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.89A From I2	4.18 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.75A From N1	4.17 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.21A From N3	4.02 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.79A From N3	3.95 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.28A From N2	3.86 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.37A From I1	3.76 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 2.28A From I1	3.72 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 0.80A From I1	3.69 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 0.62A From N1	3.67 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 2.10A From N2	3.62 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.77A From N1	-6.71 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 0.74A From I1	-6.68 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 0.83A From N3	-6.00 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 0.75A From I1	-5.96 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 2.38A From I1	-5.64 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 0.90A From I2	-4.99 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.91A From N1	-4.63 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.98A From C2	-4.46 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 0.75A From C2	-4.32 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.38A From C4	-4.22 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.90A From I2	-4.21 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.62A From N3	-4.19 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.35A From N1	-4.18 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.48A From Bi1	-4.15 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 2.25A From N1	-4.05 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 2.03A From I1	-4.05 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.63A From C1	-4.05 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 0.72A From N1	-3.97 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.02A From N1	-3.96 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.79A From I1	-3.94 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.80A From I2	-3.92 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.58A From N3	-3.92 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 0.92A From I2	-3.91 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.78A From N1	-3.90 eA-3
PLAT972_ALERT_2_A	Check Calcd Resid. Dens. 1.33A From I1	-3.86 eA-3
PLAT976_ALERT_2_A	Check Calcd Resid. Dens. 0.83A From N3	-6.00 eA-3
PLAT977_ALERT_2_A	Check Negative Difference Density on H1	-2.03 eA-3
PLAT977_ALERT_2_A	Check Negative Difference Density on H1A	-3.27 eA-3

---

## 🟡 Alert level B

PLAT925\_ALERT\_1\_B The Reported and Calculated Rho(max) Differ by . 2.22 eA-3  
PLAT939\_ALERT\_3\_B Large Value of Not (SHELXL) Weight Optimized S . 108.51 Check

---

## 🟢 Alert level C

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
PLAT043\_ALERT\_1\_C Calculated and Reported Mol. Weight Differ by .. 2.02 Check  
PLAT068\_ALERT\_1\_C Reported F000 Differs from Calcd (or Missing)... Please Check  
PLAT082\_ALERT\_2\_C High R1 Value ..... 0.13 Report  
PLAT084\_ALERT\_3\_C High wR2 Value (i.e. > 0.25) ..... 0.34 Report  
PLAT220\_ALERT\_2\_C NonSolvent Resd 2 C Ueq(max) / Ueq(min) Range 4.0 Ratio  
PLAT241\_ALERT\_2\_C High MainMol Ueq as Compared to Neighbors of C2 Check  
PLAT242\_ALERT\_2\_C Low MainMol Ueq as Compared to Neighbors of C3 Check  
PLAT420\_ALERT\_2\_C D-H Without Acceptor N1 --H1A . Please Check  
PLAT420\_ALERT\_2\_C D-H Without Acceptor N2 --H4 . Please Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 19.121 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 4.520 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report  
PLAT918\_ALERT\_3\_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check  
PLAT978\_ALERT\_2\_C Number C-C Bonds with Positive Residual Density. 0 Info

---

## 🟠 Alert level G

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and the formula from the \_atom\_site\* data.  
Atom count from \_chemical\_formula\_sum: C5 H7 Bi1 I4 N3  
Atom count from the \_atom\_site data: C5 H5 Bi1 I4 N3  
CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
CELLZ01\_ALERT\_1\_G WARNING: H atoms missing from atom site list. Is this intentional?  
From the CIF: \_cell\_formula\_units\_Z 4  
From the CIF: \_chemical\_formula\_sum C5 H7 Bi I4 N3  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	20.00	20.00	0.00
H	28.00	20.00	8.00
Bi	4.00	4.00	0.00
I	16.00	16.00	0.00
N	12.00	12.00	0.00

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 5 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report  
PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 1 Info  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 3 Report  
PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 1950.50 Why ?  
PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 1 Report  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 1 Report  
PLAT186\_ALERT\_4\_G The CIF-Embedded .res File Contains ISOR Records 4 Report  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of N1 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of N2 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C4 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H1A Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H1B Constrained at 0.5 Check  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 2 ) 38% Note  
PLAT414\_ALERT\_2\_G Short Intra D-H..H-X H1 ..H1A 1.90 Ang.  
x,y,z = 1\_555 Check  
PLAT414\_ALERT\_2\_G Short Intra D-H..H-X H1 ..H1A 1.90 Ang.  
-x,y,3/2-z = 3\_556 Check  
PLAT789\_ALERT\_4\_G Atoms with Negative \_atom\_site\_disorder\_group # 6 Check  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Bi1 (III) . 3.07 Info

PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	41	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	1	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....		Please Check
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	1	Check

---

57 **ALERT level A** = Most likely a serious problem - resolve or explain  
2 **ALERT level B** = A potentially serious problem, consider carefully  
15 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
28 **ALERT level G** = General information/check it is not something unexpected

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
66 ALERT type 2 Indicator that the structure model may be wrong or deficient  
11 ALERT type 3 Indicator that the structure quality may be low  
9 ALERT type 4 Improvement, methodology, query or suggestion  
5 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.

---

**PLATON version of 22/12/2019; check.def file version of 13/12/2019**

