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

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Bond precision:  C-C = 0.0300 A          Wavelength=0.71073

Cell:              a=12.083(4)      b=15.268(5)      c=7.876(3)
                   alpha=90         beta=90          gamma=90
Temperature:       293 K
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	Calculated	Reported
Volume	1453.0(9)	1453.0(8)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	Bi I4, C5 H7 N3	C5 H7 Bi I4 N3
Sum formula	C5 H7 Bi I4 N3	C5 H7 Bi I4 N3
Mr	825.72	825.72
Dx,g cm-3	3.775	3.775
Z	4	4
Mu (mm-1)	20.603	20.603
F000	1412.0	1412.0
F000’	1389.64	
h,k,lmax	14,18,9	14,18,9
Nref	1337	1336
Tmin,Tmax	0.050,0.127	
Tmin’	0.016	

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Correction method= Not given

Data completeness= 0.999          Theta(max)= 25.334

R(reflections)= 0.0450( 1175)     wR2(reflections)= 0.1120( 1336)

S = 1.176                 Npar= 71
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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

PLAT058_ALERT_1_A Maximum Transmission Factor Missing ..... ?
PLAT059_ALERT_1_A Minimum Transmission Factor Missing ..... ?

Alert level B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.03 Ang.
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... 1 Check

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Alert level C

PLAT213_ALERT_2_C Atom C1 has ADP max/min Ratio ..... 3.4 prolat
PLAT242_ALERT_2_C Low MainMol Ueq as Compared to Neighbors of Bi1 Check
PLAT242_ALERT_2_C Low MainMol Ueq as Compared to Neighbors of C3 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.2 Note
PLAT420_ALERT_2_C D-H Without Acceptor N1 --H1C . 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 ..... 2.463 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.90A From Bi1 2.19 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.86A From Bi1 2.02 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.82A From Bi1 1.85 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.23A From Bi1 -2.03 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.88A From Bi1 -1.76 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.89A From N3 0.93 eA-3

Alert level G

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 7.66 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
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 H1B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1C 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 ..H1C 1.88 Ang.
x,y,z = 1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X H1 ..H1C 1.88 Ang.
1-x,y,3/2-z = 4_656 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 6 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Bi1 (III) . 3.12 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 74% Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

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

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

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 16 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
  8 ALERT type 4 Improvement, methodology, query or suggestion
  3 ALERT type 5 Informative message, check
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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

Datablock shelx - ellipsoid plot