

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

Datablock: BiI3-hs3112048

Bond precision: Bi- I = 0.0100 Å Wavelength=0.41312

Cell: a=3.7558(9) b=12.101(4) c=8.957(3)
 alpha=90 beta=90 gamma=90
Temperature: 295 K

	Calculated	Reported
Volume	407.1(2)	407.1(4)
Space group	C m c m	C m c m
Hall group	-C 2c 2	?
Moiety formula	Bi I3	?
Sum formula	Bi I3	BiI3
Mr	589.68	589.67
Dx,g cm-3	9.621	9.620
Z	4	4
Mu (mm-1)	15.841	18.010
F000	968.0	968.0
F000'	943.02	
h,k,lmax	3,12,9	
Nref	141	
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.000 Theta(max)=

R(reflections)= wR2(reflections)=

S = Npar=

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

POWD002_ALERT_1_B `_refine_ls_goodness_of_fit_all` is missing (this is chi, i.e. the square root of 'chi squared'). This should be present for a powder diffraction study.

POWD004_ALERT_1_B No 'Bragg' R factor has been given. Please supply a value for `_refine_ls_R_factor_all` [R(F)], `_refine_ls_R_Fsqd_factor` [R(F²)] or `_refine_ls_R_I_factor` [R(I)].

🟢 Alert level C

REFI015_ALERT_1_C `_refine_ls_shift/su_max` is missing
Maximum shift/s.u. ratio after final refinement cycle.
The following tests will not be performed
SHFSU_01

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings	Differ	Please Check
PLAT701_ALERT_1_C	Bond Calc 3.440(13), Rep 3.423(13), Dev..			1.31 Sigma
	I2 -I2 1.555 7.556	#	25	Check
PLAT702_ALERT_1_C	Angle Calc 149.05(17), Rep 149.23(4), Dev..			1.06 Sigma
	BI -I1 -I2 9.545 1.555 13.456	#	60	Check
PLAT702_ALERT_1_C	Angle Calc 149.05(17), Rep 149.23(4), Dev..			1.06 Sigma
	BI -I1 -I2 9.445 1.555 13.556	#	72	Check
PLAT702_ALERT_1_C	Angle Calc 112.6(2), Rep 112.87(3), Dev..			1.35 Sigma
	I2 -I1 -I2 11.554 1.555 3.564	#	93	Check
PLAT702_ALERT_1_C	Angle Calc 112.6(2), Rep 112.87(3), Dev..			1.35 Sigma
	I2 -I1 -I2 11.454 1.555 3.564	#	104	Check
PLAT702_ALERT_1_C	Angle Calc 112.6(2), Rep 112.87(3), Dev..			1.35 Sigma
	I2 -I1 -I2 13.556 1.555 5.566	#	115	Check
PLAT702_ALERT_1_C	Angle Calc 112.6(2), Rep 112.87(3), Dev..			1.35 Sigma
	I2 -I1 -I2 13.456 1.555 5.566	#	124	Check
PLAT702_ALERT_1_C	Angle Calc 97.5(3), Rep 97.16(3), Dev..			1.13 Sigma
	BI -I2 -I2 1.555 1.555 5.566	#	186	Check
PLAT702_ALERT_1_C	Angle Calc 132.5(3), Rep 132.13(3), Dev..			1.23 Sigma
	I2 -I2 -I2 5.566 1.555 13.566	#	202	Check
PLAT702_ALERT_1_C	Angle Calc 132.5(3), Rep 132.13(3), Dev..			1.23 Sigma
	I2 -I2 -I2 5.566 1.555 13.466	#	203	Check
PLAT702_ALERT_1_C	Angle Calc 163.8(4), Rep 164.22(3), Dev..			1.05 Sigma
	I1 -I2 -I2 11.555 1.555 13.466	#	212	Check
PLAT702_ALERT_1_C	Angle Calc 163.8(4), Rep 164.22(3), Dev..			1.05 Sigma
	I1 -I2 -I2 11.455 1.555 13.566	#	219	Check
PLAT702_ALERT_1_C	Angle Calc 73.3(3), Rep 72.97(2), Dev..			1.10 Sigma
	I1 -I2 -I2 9.555 1.555 13.566	#	232	Check
PLAT702_ALERT_1_C	Angle Calc 105.7(3), Rep 105.35(3), Dev..			1.17 Sigma
	I1 -I2 -I2 9.555 1.555 13.466	#	233	Check
PLAT702_ALERT_1_C	Angle Calc 105.7(3), Rep 105.35(3), Dev..			1.17 Sigma
	I1 -I2 -I2 9.455 1.555 13.566	#	237	Check
PLAT702_ALERT_1_C	Angle Calc 73.3(3), Rep 72.97(2), Dev..			1.10 Sigma
	I1 -I2 -I2 9.455 1.555 13.466	#	238	Check

🟢 Alert level G

ABSMU01_ALERT_1_G Calculation of `_exptl_absorpt_correction_mu`
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.41312	Ang.
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	-2	Units
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I1 ..I2	3.35	Ang.
	1/2-x,1/2-y,-1/2+z =	12_554	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I1 ..I2	3.35	Ang.
	-1/2+x,1/2-y,1-z =	14_456	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I1 ..I2	3.35	Ang.

	$-1/2-x, 1/2-y, -1/2+z$	=	12_454	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I1	..I2	3.35	Ang.
	$1/2+x, 1/2-y, 1-z$	=	14_556	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I2	..I2	3.28	Ang.
	$x, 1-y, 1-z$	=	6_566	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I2	..I2	3.44	Ang.
	$-x, y, 3/2-z$	=	7_556	Check
PLAT984_ALERT_1_G	The I-f' =	-1.9060	Deviates from the B&C-Value	-1.9047 Check
PLAT985_ALERT_1_G	The Bi-f" =	4.4290	Deviates from the B&C-Value	4.4264 Check

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

25 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 6 ALERT type 2 Indicator that the structure model may be wrong or deficient
 0 ALERT type 3 Indicator that the structure quality may be low
 1 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 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

