

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sdab151112

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: sdab151112

Bond precision: C-C = 0.0080 A

Wavelength=0.71073

Cell: a=11.7755(10) b=19.8637(17) c=24.519(2)
 alpha=96.283(2) beta=93.717(2) gamma=90.052(2)
Temperature: 173 K

	Calculated	Reported
Volume	5688.5(8)	5688.5(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C72 H65 In N2	C72 H65 In N2
Sum formula	C72 H65 In N2	C72 H65 In N2
Mr	1073.08	1073.08
Dx,g cm-3	1.253	1.253
Z	4	4
Mu (mm-1)	0.460	0.460
F000	2240.0	2240.0
F000'	2237.79	
h,k,lmax	15,26,32	15,26,32
Nref	27635	27504
Tmin,Tmax	0.936,0.964	0.660,0.746
Tmin'	0.921	

Correction method= # Reported T Limits: Tmin=0.660 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.995

Theta(max)= 28.051

R(reflections)= 0.0886(12789)

wR2(reflections)= 0.1438(27504)

S = 0.987

Npar= 1331

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**

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.154
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.154 Report
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 46% Check
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 5.2 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 4.7 Ratio
PLAT222_ALERT_3_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 4.6 Ratio
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.00804 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 21.424 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.388 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report

● **Alert level G**

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) In1 --C70 . 11.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) In1 --C72 . 5.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) In2 --C144 . 6.4 s.u.
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 126 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

-
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected
- 1 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
9 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
-
-

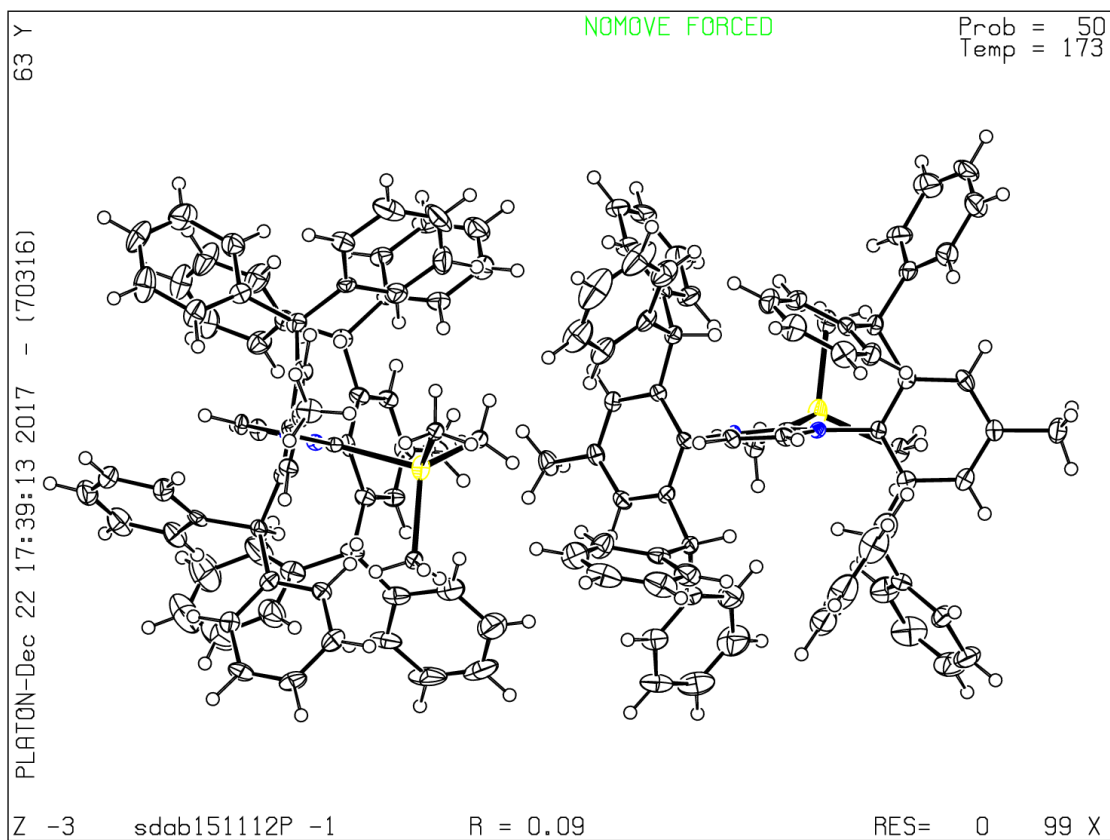
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 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.



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: rwgs120626_02

Bond precision: C-C = 0.0025 Å Wavelength=0.71073

Cell: a=9.2573(3) b=17.6283(6) c=10.1202(4)
 alpha=90 beta=90 gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	1651.52(10)	1651.52(10)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C14 H31 Ga N2	C14 H31 Ga N2
Sum formula	C14 H31 Ga N2	C14 H31 Ga N2
Mr	297.13	297.13
Dx,g cm-3	1.195	1.195
Z	4	4
Mu (mm-1)	1.652	1.652
F000	640.0	640.0
F000'	641.00	
h,k,lmax	13,25,14	13,25,14
Nref	2710	2704
Tmin,Tmax	0.615,0.719	0.558,0.734
Tmin'	0.511	

Correction method= # Reported T Limits: Tmin=0.558 Tmax=0.734
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 30.980

R(reflections)= 0.0283(2295) wR2(reflections)= 0.0710(2704)

S = 1.170 Npar= 87

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 G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Gal --C7 .	5.1 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of H8A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8C Constrained at	0.5 Check
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2017 Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
4 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

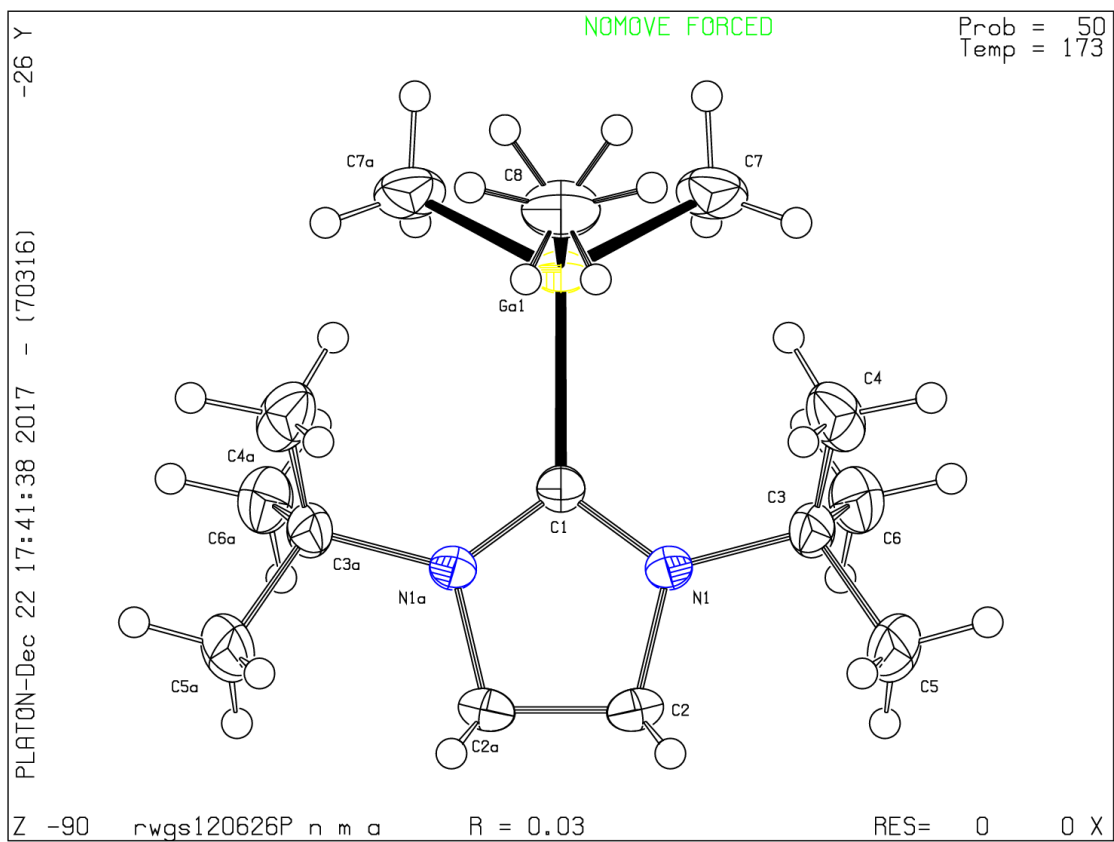
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



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: rwgs120620

Bond precision: C-C = 0.0030 Å Wavelength=0.71073

Cell: a=9.4106(6) b=17.6445(12) c=10.2584(7)
 alpha=90 beta=90 gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	1703.4(2)	1703.4(2)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C14 H31 In N2	C14 H31 In N2
Sum formula	C14 H31 In N2	C14 H31 In N2
Mr	342.23	342.23
Dx,g cm-3	1.334	1.334
Z	4	4
Mu (mm-1)	1.374	1.374
F000	712.0	712.0
F000'	709.23	
h,k,lmax	14,26,15	14,26,15
Nref	3053	3035
Tmin,Tmax	0.508,0.577	0.547,0.609
Tmin'	0.498	

Correction method= # Reported T Limits: Tmin=0.547 Tmax=0.609
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 32.040

R(reflections)= 0.0247(2680) wR2(reflections)= 0.0541(3035)

S = 1.296 Npar= 93

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

PLAT391_ALERT_3_C Deviating Methyl C8	H-C-H Bond Angle	102 Degree
PLAT391_ALERT_3_C Deviating Methyl C8	H-C-H Bond Angle	102 Degree

**Alert level G**

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF	Please Do !
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	2 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL	2017 Note

0	ALERT level A	= Most likely a serious problem - resolve or explain
0	ALERT level B	= A potentially serious problem, consider carefully
2	ALERT level C	= Check. Ensure it is not caused by an omission or oversight
3	ALERT level G	= General information/check it is not something unexpected
0	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
0	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
2	ALERT type 4	Improvement, methodology, query or suggestion
1	ALERT type 5	Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT391_rwgs120620
;
PROBLEM: Deviating Methyl C8
RESPONSE: ...
;
# end Validation Reply Form
```

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.

