

# checkCIF/PLATON report

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

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: rwhf101125

---

Bond precision:    C-C = 0.0046 Å                      Wavelength=0.71073

Cell:              a=9.9023(4)              b=11.0556(4)              c=11.6943(4)  
                    alpha=117.631(2)          beta=95.729(2)          gamma=101.957(2)

Temperature:      173 K

	Calculated	Reported
Volume	1080.91(7)	1080.91(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H32 Ga N3 O	C24 H32 Ga N3 O
Sum formula	C24 H32 Ga N3 O	C24 H32 Ga N3 O
Mr	448.25	448.25
Dx,g cm <sup>-3</sup>	1.377	1.377
Z	2	2
Mu (mm <sup>-1</sup> )	1.293	1.293
F000	472.0	472.0
F000'	472.57	
h,k,lmax	12,14,15	12,14,15
Nref	4970	4923
Tmin,Tmax	0.741,0.824	0.621,0.827
Tmin'	0.630	

Correction method= MULTI-SCAN

Data completeness= 0.991                      Theta(max)= 27.510

R(reflections)= 0.0354( 4442)              wR2(reflections)= 0.1241( 4923)

S = 1.199                                      Npar= 264

---

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

PLAT220_ALERT_2_C	Large Non-Solvent	C	Ueq(max)/Ueq(min) ...	3.1	Ratio
PLAT241_ALERT_2_C	Check High		Ueq as Compared to Neighbors for	C3	
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond	C3	- C4 ...	1.43	Ang.

---

**Alert level G**

PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in CIF .... ?  
PLAT153\_ALERT\_1\_G The su's on the Cell Axes are Equal ..... 0.00040 Ang.  
PLAT154\_ALERT\_1\_G The su's on the Cell Angles are Equal ..... 0.00200 Deg.

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
3 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 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  
0 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

---

**Datablock: rwfh111004**

---

Bond precision: C-C = 0.0047 A                      Wavelength=0.71073

Cell:                      a=10.7114(5)                      b=12.0160(5)                      c=12.5614(9)  
                            alpha=113.354(1)                      beta=107.228(1)                      gamma=103.315(1)  
Temperature: 173 K

	Calculated	Reported
Volume	1301.48(13)	1301.48(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C56 H64 Ga2 N6 O2, 2(C H2 C12)	C56 H64 Ga2 N6 O2, 2(C H2 C12)
Sum formula	C58 H68 Cl4 Ga2 N6 O2	C58 H68 Cl4 Ga2 N6 O2
Mr	1162.42	1162.42
Dx,g cm-3	1.483	1.483
Z	1	1
Mu (mm-1)	1.291	1.291
F000	604.0	604.0
F000'	605.19	
h,k,lmax	15,16,17	15,16,17
Nref	7585	7566
Tmin,Tmax	0.780,0.879	0.782,0.882
Tmin'	0.765	

Correction method= MULTI-SCAN

Data completeness= 0.997                      Theta(max)= 30.000

R(reflections)= 0.0449( 6225)                      wR2(reflections)= 0.1357( 7566)

S = 1.069

Npar= 331

---

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**

PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	C29
PLAT420_ALERT_2_C	D-H Without Acceptor	N3 - H3N ...	?

---

**Alert level G**

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF ....	?
PLAT007_ALERT_5_G	Note: Number of Unrefined D-H Atoms .....	1
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal .....	0.00100 Deg.
PLAT301_ALERT_3_G	Note: Main Residue Disorder .....	6 Perc.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	2

- 
- 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  
5 **ALERT level G** = General information/check it is not something unexpected
- 1 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  
1 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
2 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*, 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 21/12/2011; check.def file version of 16/12/2011**



