



## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 449\_tw

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: 449\_tw

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Bond precision:    C-C = 0.0145 Å

Wavelength=0.71073

Cell:                    a=8.9585(13)                    b=9.7999(14)                    c=12.979(2)  
                          alpha=82.038(4)                    beta=81.153(4)                    gamma=82.512(4)  
Temperature:           150 K

|                        | Calculated                    | Reported                      |
|------------------------|-------------------------------|-------------------------------|
| Volume                 | 1108.1(3)                     | 1108.1(3)                     |
| Space group            | P -1                          | P -1                          |
| Hall group             | -P 1                          | -P 1                          |
| Moiety formula         | C8 H22 B2 Ga N4 O5, B5 H4 O10 | C8 H22 B2 Ga N4 O5, B5 H4 O10 |
| Sum formula            | C8 H26 B7 Ga N4 O15           | C8 H26 B7 Ga N4 O15           |
| Mr                     | 563.72                        | 563.72                        |
| Dx, g cm <sup>-3</sup> | 1.689                         | 1.689                         |
| Z                      | 2                             | 2                             |
| Mu (mm <sup>-1</sup> ) | 1.321                         | 1.321                         |
| F000                   | 576.0                         | 576.0                         |
| F000'                  | 576.77                        |                               |
| h, k, lmax             | 10, 11, 15                    | 10, 11, 15                    |
| Nref                   | 3992                          | 3941                          |
| Tmin, Tmax             |                               |                               |
| Tmin'                  |                               |                               |

Correction method= Not given

Data completeness= 0.987

Theta(max)= 25.175

R(reflections)= 0.0845( 2902)

wR2(reflections)=  
0.2484( 3941)

S = 1.059

Npar= 323

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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.

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#### Alert level C

|                   |                                                       |              |
|-------------------|-------------------------------------------------------|--------------|
| PLAT018_ALERT_1_C | _diffraction_measured_fraction_theta_max .NE. *_full  | ! Check      |
| PLAT053_ALERT_1_C | Minimum Crystal Dimension Missing (or Error) ...      | Please Check |
| PLAT054_ALERT_1_C | Medium Crystal Dimension Missing (or Error) ...       | Please Check |
| PLAT055_ALERT_1_C | Maximum Crystal Dimension Missing (or Error) ...      | Please Check |
| PLAT241_ALERT_2_C | High MainResAtom Ueq as Compared to Neighbours        | C1 Check     |
| PLAT341_ALERT_3_C | Low Bond Precision on C-C Bonds .....                 | 0.0145 Ang.  |
| PLAT420_ALERT_2_C | D-H Bond Without Acceptor N1 --H1 .                   | Please Check |
| PLAT420_ALERT_2_C | D-H Bond Without Acceptor N2 --H2 .                   | Please Check |
| PLAT906_ALERT_3_C | Large K Value in the Analysis of Variance .....       | 6.422 Check  |
| PLAT911_ALERT_3_C | Missing FCF Refl Between Thmin & STh/L= 0.597         | 21 Report    |
|                   | -7 -5 1, 6 -5 1, -2 -1 1, -10 -2 3, -10 0 3, -9 -5 4, |              |
|                   | 0 -3 4, -6 -8 5, -9 -2 6, -9 1 6, 4 11 6, 1 3 7,      |              |
|                   | -7 0 10, 0 -7 11, 4 -6 11, -5 -2 12, -5 3 12, 2 7 13, |              |
|                   | 1 -2 14, 5 5 14, -1 1 15,                             |              |



#### Alert level G

|                   |                                                            |              |
|-------------------|------------------------------------------------------------|--------------|
| PLAT007_ALERT_5_G | Number of Unrefined Donor-H Atoms .....                    | 10 Report    |
|                   | H1 H2 H3 H3A H4 H5 H6 H8                                   |              |
|                   | H13 H15                                                    |              |
| PLAT072_ALERT_2_G | SHELXL First Parameter in WGHT Unusually Large             | 0.16 Report  |
| PLAT154_ALERT_1_G | The s.u.'s on the Cell Angles are Equal ..(Note)           | 0.004 Degree |
| PLAT870_ALERT_4_G | ALERTS Related to Twinning Effects Suppressed ..           | ! Info       |
| PLAT909_ALERT_3_G | Percentage of I>2sig(I) Data at Theta(Max) Still           | 41% Note     |
| PLAT910_ALERT_3_G | Missing FCF Reflection(s) Below Theta(Min) [Deg]=          | 2.11 Note    |
|                   | 0 0 1,                                                     |              |
| PLAT931_ALERT_5_G | CIFcalcFCF Twin Law ( 1 0 0) Est.d BASF                    | 0.19 Check   |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity .....                 | 1.0 Low      |
| PLAT961_ALERT_5_G | Dataset Contains no Negative Intensities .....             | Please Check |
| PLAT969_ALERT_5_G | The 'Henn et al.' R-Factor-gap value .....                 | 4.899 Note   |
|                   | Predicted wR2: Based on SigI**2 5.07 or SHELX Weight 23.46 | Note         |
| PLAT994_ALERT_1_G | SHELXL .ins with Im-/Explicit MERG 0 Instruction           | ! Note       |

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- 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  
11 **ALERT level G** = General information/check it is not something unexpected
- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

4 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  
1 ALERT type 4 Improvement, methodology, query or suggestion  
4 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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**PLATON version of 23/04/2026; check.def file version of 30/03/2026**

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## **duplicate check**

**No duplication found**

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