

# checkCIF/PLATON report

No syntax errors found.    CIF dictionary    Interpreting this report

## Datablock: DC133

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Bond precision:    C-C = 0.0025 A

Wavelength=0.71073

Cell:                    a=11.4688(12)            b=22.418(2)            c=10.6590(12)

                          alpha=90                    beta=90                    gamma=90

Temperature:            150 K

	Calculated	Reported
Volume	2740.5(5)	2740.5(5)
Space group	C c c 2	C c c 2
Hall group	C 2 -2c	C 2 -2c
Moiety formula	C24 H26 Br2 O6 Ti	C12 H13 Br O3 Ti0.5
Sum formula	C24 H26 Br2 O6 Ti	C12 H13 Br O3 Ti0.5
Mr	618.12	309.07
Dx,g cm-3	1.498	1.498
Z	4	8
Mu (mm-1)	3.262	3.261
F000	1240.0	1239.6
F000'	1239.39	
h,k,lmax	17,34,16	17,34,16
Nref	5410[ 2832]	5371
Tmin,Tmax		0.690,0.747
Tmin'		

Correction method= MULTI-SCAN

Data completeness= 1.90/0.99

Theta(max)= 33.550

R(reflections)= 0.0281( 4531)

wR2(reflections)= 0.0714( 5371)

S = 0.964

Npar= 151

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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

PLAT041_ALERT_1_C Calc. and Reported SumFormula	Strings Differ	Please 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
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .		37 Ang3

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## ● Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by .....	0.50 Ratio
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	13
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Til -- O1 ..	5.8 su
PLAT982_ALERT_1_G	The Br-f' = -0.283 Deviates from the IT-value	-0.290
PLAT982_ALERT_1_G	The Ti-f' = 0.291 Deviates from the IT-value	0.278
PLAT983_ALERT_1_G	The Br-f" = 2.560 Deviates from the IT-Value	2.460

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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  
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
7 **ALERT level G** = General information/check it is not something unexpected

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 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  
0 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*, 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.

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