

# 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: I

---

Bond precision:	C-C = 0.0058 A	Wavelength=0.71075	
Cell:	a=13.933(4)	b=14.981(4)	c=14.835(4)
	alpha=90	beta=107.809(3)	gamma=90
Temperature:	103 K		
	Calculated	Reported	
Volume	2948.1(14)	2948.1(13)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C42 H40 B4 Cl2 N24 O4 Tb2, 2(C H2 Cl2)	C42 H40 B4 Cl2 N24 O4 Tb2, 2(C H2 Cl2)	
Sum formula	C44 H44 B4 Cl6 N24 O4 Tb2	C44 H44 B4 Cl6 N24 O4 Tb2	
Mr	1546.83	1546.80	
Dx,g cm-3	1.742	1.742	
Z	2	2	
Mu (mm-1)	2.716	2.710	
F000	1520.0	1520.0	
F000'	1521.42		
h,k,lmax	18,19,19	18,19,19	
Nref	6748	6740	
Tmin,Tmax	0.392,0.582	0.441,0.582	
Tmin'	0.248		

Correction method= # Reported T Limits: Tmin=0.441 Tmax=0.582  
AbsCorr = MULTI-SCAN

Data completeness= 0.999      Theta(max)= 27.466

R(reflections)= 0.0354( 5830)      wR2(reflections)= 0.0684( 6740)

S = 1.069      Npar= 379

---

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**  
PLAT369\_ALERT\_2\_C Long C(sp2)-C(sp2) Bond C1 - C2 . 1.54 Ang.

---

 **Alert level G**  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 8.34 Why ?  
PLAT333\_ALERT\_2\_G Large Aver C6-Ring C-C Dist C1 -C3\_a . 1.44 Ang.  
PLAT335\_ALERT\_2\_G Check Large C6 Ring C-C Range C1 -C3\_a 0.15 Ang.  
PLAT790\_ALERT\_4\_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note  
C H2 C12  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Tb1 (III) . 3.53 Info  
PLAT882\_ALERT\_1\_G No Datum for \_diffrn\_reflms\_av\_unetI/netI ..... Please Do !

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
1 **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

1 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  
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

---

## Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

---

**PLATON version of 13/12/2018; check.def file version of 11/12/2018**

