

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) A21127O\_004

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: A21127O\_004

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Bond precision:    C-C = 0.0088 A                      Wavelength=0.71073

Cell:                      a=11.8606(8)              b=17.7171(11)              c=12.5793(8)  
                            alpha=90                      beta=98.8655(18)              gamma=90

Temperature:            173 K

	Calculated	Reported
Volume	2611.8(3)	2611.8(3)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C23 H27 B10 Br O2	C23 H27 B10 Br O2
Sum formula	C23 H27 B10 Br O2	C23 H27 B10 Br O2
Mr	523.45	523.45
Dx,g cm-3	1.331	1.331
Z	4	4
Mu (mm-1)	1.595	1.595
F000	1064.0	1064.0
F000'	1063.16	
h,k,lmax	14,22,15	14,22,15
Nref	10819[ 5590]	10783
Tmin,Tmax	0.905,0.955	0.424,0.746
Tmin'	0.624	

Correction method= # Reported T Limits: Tmin=0.424 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 1.93/1.00                      Theta(max)= 26.493

R(reflections)= 0.0476( 7474)                      wR2(reflections)= 0.1150( 10783)

S = 1.020                                      Npar= 668

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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**

PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00882 Ang.
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	6 Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	4 Report

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**Alert level G**

PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	4 Note
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C1A Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C2A Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C1B Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C2B Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1A - C2A	1.65 Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1A - C13A	1.52 Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1B - C2B	1.64 Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1B - C13B	1.52 Ang.
PLAT791_ALERT_4_G	Model has Chirality at C14A (Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G	Model has Chirality at C14B (Sohnke SpGr)	R Verify
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	3 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
9 ALERT type 2 Indicator that the structure model may be wrong or deficient  
4 ALERT type 3 Indicator that the structure quality may be low  
3 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* 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.

