

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ABX15

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: ABX15

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Bond precision:    C-C = 0.0036 A                      Wavelength=0.71073

Cell:                      a=6.2993(9)              b=19.436(3)              c=14.739(2)  
                                    alpha=90              beta=91.626(7)              gamma=90

Temperature:              295 K

	Calculated	Reported
Volume	1803.8(5)	1803.8(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C22 H18 N2 O3	C22 H18 N2 O3
Sum formula	C22 H18 N2 O3	C22 H18 N2 O3
Mr	358.38	358.38
Dx,g cm-3	1.320	1.320
Z	4	4
Mu (mm-1)	0.089	0.089
F000	752.0	752.0
F000'	752.34	
h,k,lmax	9,29,22	9,27,20
Nref	6518	5350
Tmin,Tmax	0.991,0.996	0.648,0.746
Tmin'	0.988	

Correction method= # Reported T Limits: Tmin=0.648 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.821                      Theta(max)= 32.490

R(reflections)= 0.0742( 3188)              wR2(reflections)= 0.2408( 5350)

S = 1.044                      Npar= 245

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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**

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full	value Low	.	0.964	Note
PLAT220_ALERT_2_C	Non-Solvent Resd	1	C Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C21	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C12	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C16	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C22	Check
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond	C20 - C21 ..	1.38	Ang.
PLAT410_ALERT_2_C	Short	Intra H...H Contact	H20A .. H21A ..	1.95	Ang.
PLAT410_ALERT_2_C	Short	Intra H...H Contact	H20B .. H21B ..	1.96	Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	.....		10.929	Check
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	.....		3.053	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min)			8	Note
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600		105	Report
PLAT977_ALERT_2_C	Check the Negative Difference Density on	H21A		-0.36	eA-3

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● **Alert level G**

PLAT005_ALERT_5_G	No Embedded Refinement Details found	in the CIF		Please Do !
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT	Unusually Large		0.12 Report
PLAT343_ALERT_2_G	Unusual sp3	Angle Range in Main Residue for		C21 Check
PLAT793_ALERT_4_G	The Model has Chirality at C9	(Centro SPGR)		R Verify
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		961 Note
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported	Kmax Differ		2 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported	Lmax Differ		2 Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF)	Kmax Differ		2 Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF)	Lmax Differ		2 Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			6 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  
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
10 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
12 ALERT type 2 Indicator that the structure model may be wrong or deficient  
5 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
3 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.

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**PLATON version of 24/11/2016; check.def file version of 23/11/2016**

