

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB4a

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: MAB4a

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Bond precision:      C-C = 0.0014 A

Wavelength=0.71075

Cell:                      a=9.0534 (1)                      b=11.9367 (2)                      c=14.5824 (2)  
                                    alpha=94.195 (1)                      beta=104.156 (1)                      gamma=94.855 (1)  
Temperature:              100 K

	Calculated	Reported
Volume	1515.35 (4)	1515.35 (4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H34 N2, 2 (B5 H4 O10)	C16 H34 N2, 2 (B5 H4 O10)
Sum formula	C16 H42 B10 N2 O20	C16 H42 B10 N2 O20
Mr	690.62	690.61
Dx, g cm <sup>-3</sup>	1.514	1.514
Z	2	2
Mu (mm <sup>-1</sup> )	0.127	0.127
F000	724.0	724.0
F000'	724.48	
h, k, lmax	11, 15, 18	11, 15, 18
Nref	6958	6954
Tmin, Tmax	0.972, 0.985	0.757, 1.000
Tmin'	0.972	

Correction method= # Reported T Limits: Tmin=0.757 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta (max)= 27.484

R(reflections)= 0.0314 ( 6407)

wR2(reflections)=  
0.0906 ( 6954)

S = 1.044

Npar= 443

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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**

PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem	I	95 %Fit
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	3 Report
	-1 2 1, -1 0 3, 0 0 4,		

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**Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....		8 Report
	H7 H8 H9 H10 H17 H18 H19 H20		
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.001 Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....		33 Note
	Hb Hc Hr Hs H1AA H2AA Ha Hv		
	Hw Hp Hq Hd He Hf Hg Hx		
	Hy Ht Hu H0AA Hz H5AA H6AA H3AA		
	H4AA Hn Ho Hk Hl Hm Hh Hi		
	Hj		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2 Note
	B5 H4 O10		
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1 Note
	0 0 1,		
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....		3 Note
	-1 2 1, -1 0 3, 0 0 4,		
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....		5.54 Note
	Predicted wR2: Based on SigI**2 1.63 or SHELX Weight	8.97	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		7 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  
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
8 **ALERT level G** = General information/check it is not something unexpected

1 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  
3 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

