

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB8

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: MAB8

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Bond precision:    C-C = 0.0016 A

Wavelength=0.71075

Cell:                    a=26.8754(5)            b=11.5269(2)            c=17.9383(4)  
                          alpha=90            beta=103.154(2)        gamma=90  
Temperature:            100 K

	Calculated	Reported
Volume	5411.30(19)	5411.30(19)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	4(B5 H4 O10), 2(C9 H24 N2), H2 O	C9 H24 N2, 2(B5 H4 O10), 0.5(H2 O)
Sum formula	C18 H66 B20 N4 O41	C9 H33 B10 N2 O20.50
Mr	1210.95	605.47
Dx,g cm-3	1.486	1.486
Z	4	8
Mu (mm-1)	0.132	0.132
F000	2520.0	2520.0
F000'	2521.81	
h,k,lmax	34,14,23	34,14,23
Nref	6197	6191
Tmin,Tmax	0.978,0.995	0.732,1.000
Tmin'	0.966	

Correction method= # Reported T Limits: Tmin=0.732 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 27.482

R(reflections)= 0.0351( 5188)

wR2(reflections)= 0.0919( 6191)

S = 1.029

Npar= 409

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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

PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	022	0.124	Check
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H21A	..018	2.66	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....	2.383	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	3	Report

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### ● Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	.....	12	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ			Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor	...	0.50	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4 )		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5 )		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	..... Resd 4	0.79	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	..... Resd 5	0.71	Check
PLAT417_ALERT_2_G	Short Inter D-H..H-D	H8 ..H22A	2.10	Ang.
		x,-y,-1/2+z =	6_555	Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group	#	3	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	.....	1	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		3	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	....	2	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		2	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

4 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

3 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

6 ALERT type 4 Improvement, methodology, query or suggestion

1 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.

