

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB7

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: MAB7

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Bond precision:	O- B = 0.0015 A	Wavelength=1.54178
Cell:	a=9.5405(1)	b=16.1031(2)      c=9.4328(1)
	alpha=90	beta=90.171(1)      gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	1449.17(3)	1449.17(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	B5 H4 O10, C6 H14 N	B5 H4 O10, 1(C6 H14 N)
Sum formula	C6 H18 B5 N O10	C6 H18 B5 N O10
Mr	318.26	318.26
Dx,g cm-3	1.459	1.459
Z	4	4
Mu (mm-1)	1.096	1.096
F000	664.0	664.0
F000'	666.61	
h,k,lmax	11,19,11	11,19,11
Nref	2662	2661
Tmin,Tmax	0.858,0.957	0.906,1.000
Tmin'	0.858	

Correction method= # Reported T Limits: Tmin=0.906 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.000      Theta(max)= 68.183

R(reflections)= 0.0314( 2427)      wR2(reflections)= 0.0845( 2661)

S = 1.068      Npar= 271

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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.





### Alert level C

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PLAT088_ALERT_3_C	Poor Data / Parameter Ratio .....	9.82	Note
PLAT221_ALERT_2_C	Solv./Anion Resd 4 C Ueq(max)/Ueq(min) Range	4.1	Ratio
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....	2.1	Note

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### Alert level G

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PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	21	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	21	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	4	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	7	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4 )	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 2	10.19	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 3	6.13	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 4	4.68	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	26	Note
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1	Info
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	562	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  
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
17 **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  
2 ALERT type 3 Indicator that the structure quality may be low  
11 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.



