

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB2

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: MAB2

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Bond precision:      C-C = 0.0028 Å

Wavelength=0.71075

Cell:                      a=9.4616(4)                      b=9.4780(3)                      c=19.8856(8)  
                              alpha=86.483(3)                      beta=81.244(3)                      gamma=75.624(3)  
Temperature:              100 K

	Calculated	Reported
Volume	1706.79(12)	1706.79(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H28 N4, 2(B5 H4 O10), 3(H2 O)	C16 H28 N4, 2(B5 H4 O10), 3(H2 O)
Sum formula	C16 H42 B10 N4 O23	C16 H42 B10 N4 O23
Mr	766.64	766.63
Dx, g cm <sup>-3</sup>	1.492	1.492
Z	2	2
Mu (mm <sup>-1</sup> )	0.129	0.129
F000	800.0	800.0
F000'	800.54	
h,k,lmax	12,12,25	12,12,25
Nref	7833	7820
Tmin,Tmax	0.985,0.999	0.609,1.000
Tmin'	0.965	

Correction method= # Reported T Limits: Tmin=0.609 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta(max)= 27.484

R(reflections)= 0.0457( 5988)

wR2(reflections)=  
0.1431( 7820)

S = 0.970

Npar= 537

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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 B

PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O23 --H23A . Please Check

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#### Alert level C

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 3.753 Check

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#### Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 16 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 5 Report  
PLAT007\_ALERT\_3\_G Number of Unrefined Donor-H Atoms ..... 10 Report  
H21A H21B H22A H22B H22C H22D H23A H23B H23C H23D  
PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 1 Report  
PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 2 Report  
PLAT187\_ALERT\_4\_G The CIF-Embedded .res File Contains RIGU Records 1 Report  
PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0025 Report  
PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0025 Report  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O22 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H22A Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H22B Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O22A Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H22C Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H22D Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O23 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H23A Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H23B Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O23A Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H23C Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H23D Constrained at 0.5 Check  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 100% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 100% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 7) 100% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 8) 100% Note  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 5) 1.50 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 6) 1.50 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 7) 1.50 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 8) 1.50 Check  
PLAT415\_ALERT\_2\_G Short Inter D-H..H-X H12 ..H23A . 2.10 Ang.  
x,1+y,z = 1\_565 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O10 ..C14 . 2.98 Ang.  
x,y,z = 1\_555 Check  
PLAT726\_ALERT\_2\_G H...A Calc 1.94000, Rep 1.93000 Dev... 0.01 Ang.  
H21B -O22 1\_555 1\_555 ..... # 12 Check  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 21 Note  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note  
0 0 1,  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 12 Note  
PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 4.9 Low

PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 4.52 Note  
 Predicted wR2: Based on SigI\*\*2 3.17 or SHELX Weight 15.28  
 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  
 1 **ALERT level B** = A potentially serious problem, consider carefully  
 1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 38 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 7 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 6 ALERT type 3 Indicator that the structure quality may be low  
 24 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.

