

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB3

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: MAB3

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Bond precision:    C-C = 0.0020 A                      Wavelength=0.71075

Cell:              a=8.6570(3)              b=9.7443(3)              c=10.2101(3)  
                    alpha=107.087(3)      beta=102.747(3)      gamma=95.002(3)  
Temperature:      100 K

	Calculated	Reported
Volume	792.23(5)	792.23(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(B5 H4 O10), C8 H28 N4 Ni O2, 2(H2 O)	C8 H28 N4 Ni O2, 2(B5 H4 O10), 2(H2 O)
Sum formula	C8 H40 B10 N4 Ni O24	C8 H40 B10 N4 Ni O24
Mr	743.23	743.25
Dx, g cm <sup>-3</sup>	1.558	1.558
Z	1	1
Mu (mm <sup>-1</sup> )	0.708	0.708
F000	386.0	386.0
F000'	386.59	
h,k,lmax	11,12,13	11,12,13
Nref	3645	3628
Tmin,Tmax	0.850,0.945	0.892,1.000
Tmin'	0.850	

Correction method= # Reported T Limits: Tmin=0.892 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.995                      Theta(max)= 27.481

R(reflections)= 0.0270( 3568)              wR2(reflections)= 0.0731( 3628)

S = 1.088                      Npar= 225

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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**

PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....	2.3	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	7	Report
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.73A From O21	0.41	eA-3

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**Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	10	Report
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ		Please Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003	Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Nil --N12 .	5.8	s.u.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	3	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Nil (II) .	1.88	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	11	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.6	Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	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  
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
12 **ALERT level G** = General information/check it is not something unexpected

2 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  
4 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 13/07/2021; check.def file version of 13/07/2021**

