

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB6

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: MAB6

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Bond precision:    O- B = 0.0021 A                      Wavelength=0.71075

Cell:                      a=22.3539(4)              b=11.0192(2)              c=22.8834(4)  
                            alpha=90                      beta=107.630(2)              gamma=90  
Temperature:              100 K

	Calculated	Reported
Volume	5371.95(18)	5371.94(18)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C12 H32 N4 Ni O2, C12 H28 N4 Ni, 2(B7 H5 O14), 4(H2 O)	C6 H16 N2 Ni0.5 O, C6 H14 N2 Ni0.5, B7 H5 O14, 2(H2 O)
Sum formula	C24 H78 B14 N8 Ni2 O34	C12 H39 B7 N4 Ni O17
Mr	1291.66	645.85
Dx, g cm-3	1.597	1.597
Z	4	8
Mu (mm-1)	0.806	0.806
F000	2704.0	2704.0
F000'	2708.23	
h,k,lmax	28,14,29	28,14,29
Nref	6161	6154
Tmin,Tmax	0.886,0.930	0.931,1.000
Tmin'	0.886	

Correction method= # Reported T Limits: Tmin=0.931 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.999                      Theta(max)= 27.483

R(reflections)= 0.0384( 5759)              wR2(reflections)= 0.1087( 6154)

S = 1.051                      Npar= 519

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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 B

PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O14 --H14 . Please Check

### Alert level C

PLAT223_ALERT_4_C	Solv./Anion Resd 2 H Ueq(max)/Ueq(min) Range	4.1	Ratio
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare) .....	01	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.015	Check
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.96A From O23	0.45	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.98A From O21	-0.44	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H21A	-0.32	eA-3

### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	32	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	54	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	27	Report
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ	Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	14.01	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	3	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	5	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	84%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )	94%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	14	Note
PLAT793_ALERT_4_G	Model has Chirality at C1 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C2 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C11 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C12 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C1B (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C2B (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C11B (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C12B (Centro SPGR)	R	Verify
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	1247	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	3	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 1 **ALERT level B** = A potentially serious problem, consider carefully  
 6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 27 **ALERT level G** = General information/check it is not something unexpected

2 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
 9 **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  
 17 **ALERT type 4** Improvement, methodology, query or suggestion  
 2 **ALERT type 5** Informative message, check

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.

