

# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: JC011X2

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Bond precision:	C-C = 0.0023 Å	Wavelength=0.71073	
Cell:	a=15.8029(9)	b=15.8029(9)	c=16.875(2)
	alpha=90	beta=90	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	4214.2(7)	4214.3(11)	
Space group	I 41/a c d	I 41/a c d	
Hall group	-I 4bd 2c	-I 4bd 2c	
Moiety formula	C20 H20 Cl2 N4 Ni, 0.366(O), 0.733(H)	C20 H20 Cl2 N4 Ni, 0.366(H2 O)	
Sum formula	C20 H20.73 Cl2 N4 Ni O0.37	C20 H20.73 Cl2 N4 Ni O0.37	
Mr	452.58	452.61	
Dx,g cm-3	1.427	1.427	
Z	8	8	
Mu (mm-1)	1.188	1.188	
F000	1869.3	1869.0	
F000'	1874.76		
h,k,lmax	20,20,21	20,20,21	
Nref	1212	1212	
Tmin,Tmax	0.640,0.709	0.494,0.709	
Tmin'	0.485		

Correction method= # Reported T Limits: Tmin=0.494 Tmax=0.709  
AbsCorr = MULTI-SCAN

Data completeness= 1.000      Theta(max)= 27.460

R(reflections)= 0.0256( 1099)      wR2(reflections)= 0.0686( 1212)

S = 1.090      Npar= 72

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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

PLAT077\_ALERT\_4\_C Unitcell contains non-integer number of atoms .. Please Check



### Alert level G

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.

CELLZ01\_ALERT\_1\_G ALERT: check formula stoichiometry or atom site occupancies.

From the CIF: \_cell\_formula\_units\_Z 8

From the CIF: \_chemical\_formula\_sum C20 H20.73 Cl2 N4 Ni O0.37

TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	160.00	160.00	0.00
H	165.84	165.86	-0.02
Cl	16.00	16.00	0.00
N	32.00	32.00	0.00
Ni	8.00	8.00	0.00
O	2.96	2.93	0.03

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	5.08 Why ?
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...	-4 Units
PLAT300_ALERT_4_G Atom Site Occupancy of <H1 is Constrained at	0.1832 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)..	100 % Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms ( 0.09) in Resd. #	2 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms ( 0.18) in Resd. #	3 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....	01 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact Cl1 .. O1 ..	3.14 Ang.
PLAT431_ALERT_2_G Short Inter HL..A Contact Cl1 .. O1 ..	3.14 Ang.

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

- 6 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
- 0 ALERT type 3 Indicator that the structure quality may be low
- 5 ALERT type 4 Improvement, methodology, query or suggestion
- 0 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.

