

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: d504

Bond precision:	C-C = 0.0078 A	Wavelength=0.71073	
Cell:	a=30.0337(6)	b=30.0337(6)	c=11.4332(4)
	alpha=90	beta=90	gamma=90
Temperature:	294 K		
	Calculated	Reported	
Volume	10313.0(5)	10312.9(5)	
Space group	I 41/a	I 41/a	
Hall group	-I 4ad	-I 4ad	
Moiety formula	C40 H46 N4 Ni3 O16, 2(C H4 O) [+ solvent]	C40 H46 N4 Ni3 O16, 2(C H4 O)	
Sum formula	C42 H54 N4 Ni3 O18 [+ solvent]	C42 H54 N4 Ni3 O18	
Mr	1078.96	1079.02	
Dx, g cm ⁻³	1.390	1.390	
Z	8	0	
Mu (mm ⁻¹)	1.155	1.155	
F000	4496.0	4496.0	
F000'	4506.21		
h,k,lmax	37,37,14	40,40,15	
Nref	5072	5038	
Tmin,Tmax	0.724,0.785	0.748,1.000	
Tmin'	0.653		

Correction method= # Reported T Limits: Tmin=0.748 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 26.010

R(reflections)= 0.0606(3408) wR2(reflections)= 0.1842(5038)

S = 1.086 Npar= 312

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**

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.61	Report
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C4 Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00781	Ang.

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O2	111.6	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O3	111.7	Degree
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	316	A**3
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	17	Note
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	-3	Units
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	-3	Units

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
13 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
5 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

PLATON version of 30/01/2018; check.def file version of 30/01/2018

