

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: d506

Bond precision:	C-C = 0.0102 A	Wavelength=0.71073	
Cell:	a=12.3164(7)	b=13.3441(6)	c=15.2621(8)
	alpha=90	beta=111.426(7)	gamma=90
Temperature:	294 K		
	Calculated	Reported	
Volume	2335.0(2)	2335.0(2)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C44 H50 N4 Ni3 O16	C44 H50 N4 Ni3 O16	
Sum formula	C44 H50 N4 Ni3 O16	C44 H50 N4 Ni3 O16	
Mr	1066.95	1067.01	
Dx,g cm-3	1.518	1.518	
Z	2	2	
Mu (mm-1)	1.272	1.272	
F000	1108.0	1108.0	
F000'	1110.52		
h,k,lmax	15,16,18	15,16,18	
Nref	4605	4595	
Tmin,Tmax	0.664,0.709	0.934,1.000	
Tmin'	0.651		

Correction method= # Reported T Limits: Tmin=0.934 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 26.018

R(reflections)= 0.0607(2941) wR2(reflections)= 0.1662(4595)

S = 1.037 Npar= 308

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

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O3	--C9	.	5.9 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C3	--C4		0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C20	--C21		0.16 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of				O2 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of				O3 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of				C4 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of				N2 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of				C8 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of				C18 Check
PLAT341_ALERT_3_C	Low Bond Precision on	C-C Bonds		0.01017 Ang.

● Alert level G

PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for			C20 Check
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for	O2		112.6 Degree
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for	O3		115.2 Degree

- 0 ALERT level A = Most likely a serious problem - resolve or explain
 - 0 ALERT level B = A potentially serious problem, consider carefully
 - 10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 - 3 ALERT level G = General information/check it is not something unexpected
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- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 10 ALERT type 2 Indicator that the structure model may be wrong or deficient
 - 1 ALERT type 3 Indicator that the structure quality may be low
 - 2 ALERT type 4 Improvement, methodology, query or suggestion
 - 0 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.

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

Datablock d506 - ellipsoid plot

