



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 111

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: 111

Bond precision: C-C = 0.0035 Å

Wavelength=0.71073

Cell: a=9.7077 (4) b=12.9884 (5) c=14.5148 (6)
 alpha=111.098 (1) beta=95.471 (1) gamma=107.002 (1)
Temperature: 150 K

	Calculated	Reported
Volume	1591.02 (11)	1591.02 (11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H19 N4 Ni O2, B5 H4 O10, C5 H5 N	C22 H19 N4 Ni O2, B5 H4 O10, C5 H5 N
Sum formula	C27 H28 B5 N5 Ni O12	C27 H28 B5 N5 Ni O12
Mr	727.28	727.30
Dx, g cm ⁻³	1.518	1.518
Z	2	2
Mu (mm ⁻¹)	0.681	0.681
F000	748.0	748.0
F000'	749.04	
h, k, lmax	12, 16, 18	12, 16, 18
Nref	6548	6533
Tmin, Tmax	0.885, 0.922	0.011, 0.028
Tmin'	0.873	

Correction method= # Reported T Limits: Tmin=0.011 Tmax=0.028
AbsCorr = NONE

Data completeness= 0.998

Theta(max)= 26.441

R(reflections)= 0.0349(5178)

wR2(reflections)=
0.0829(6533)

S = 1.023

Npar= 456

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 G			
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4	Report
	H3A H5A H10A H12A		
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001	Degree
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit-Cell: Resd. #	3	Note
	C5 H5 N		
PLAT794_ALERT_5_G	Tentative Bond Valency for Nil (II) .	2.03	Info
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=	2.25	Note
	0 1 0, 0 -1 1, 0 0 1,		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	12	Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	2.700	Note
	Predicted wR2: Based on SigI**2 3.07 or SHELX Weight	8.10	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	5	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
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 23/04/2026; check.def file version of 30/03/2026

duplicate check

No duplication found

Datablock 111 - ellipsoid plot

