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: C5

Bond precision: C-C = 0.0068 A   Wavelength=0.71073

Cell: a=10.025(2)   b=15.265(3)   c=15.621(3)
               alpha=116.90(3)   beta=99.47(3)   gamma=92.74(3)
Temperature: 173 K

	Calculated	Reported
Volume	2082.4(10)	2082.4(7)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C44 H40 Br2 N2 Ni O, C4 H10 O	?
Sum formula	C48 H50 Br2 N2 Ni O2	C48 H50 Br2 N2 Ni O2
Mr	905.39	905.43
Dx,g cm-3	1.444	1.444
Z	2	2
Mu (mm-1)	2.426	2.426
F000	932.0	932.0
F000'	931.82	
h,k,lmax	13,19,20	13,19,20
Nref	9588	9486
Tmin,Tmax	0.445,0.631	0.710,1.000
Tmin'	0.411	

Correction method= # Reported T Limits: Tmin=0.710 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.989   Theta(max)= 27.540

R(reflections)= 0.0660(8439)   wR2(reflections)= 0.1894(9486)

S = 1.194   Npar= 504

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 Without Acceptor   O1   -   H1A   ..   Please Check

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🟡 Alert level C
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.0068 Ang.

⚪ Alert level G
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF   Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   2 Report
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .   mixed Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...   3 Units
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal .... 0.03000 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Br2   --   Ni1   ..   5.8 su
PLAT793_ALERT_4_G The Model has Chirality at C32   (Centro SPGR)   R Verify
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL   2014 Note

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   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   1 **ALERT level B** = A potentially serious problem, consider carefully
   1 **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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 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
   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*, 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 21/06/2015; check.def file version of 21/06/2015

NOMOVE FORCED

Prob = 50
Temp = 173

48 Y

PLATON-Sep 12 02:49:03 2015 - (210615)

Z 73   C5   P-1   R = 0.07   RES=   0   -88 X