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: ad56

Bond precision: C-C = 0.0038 A Wavelength=0.71073

Cell: a=10.6278(15) b=17.806(2) c=9.7465(13)
alpha=96.093(16) beta=90.759(17) gamma=102.995(16)
Temperature: 160 K

	Calculated	Reported
Volume	1785.7(4)	1785.7(4)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	4(C15 H20 N3 Ni O2), 4(Cl O4), C H O	?
Sum formula	C61 H81 Cl4 N12 Ni4 O25	C15.25 H21 Cl N3 Ni O6.25
Mr	1758.94	440.51
Dx,g cm-3	1.636	1.639
Z	1	4
Mu (mm-1)	1.276	1.276
F000	911.0	914.0
F000’	913.33	
h,k,lmax	12,20,11	12,20,11
Nref	5756	5334
Tmin,Tmax	0.638,0.880	0.617,0.878
Tmin’	0.594	

Correction method= # Reported T Limits: Tmin=0.617 Tmax=0.878
AbsCorr = NUMERICAL

Data completeness= 0.927 Theta(max)= 24.190

R(reflections)= 0.0287(4183) wR2(reflections)= 0.0611(5334)

S = 0.933 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 A

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.927 Why?
PLAT183_ALERT_1_A Missing _cell_measurement_reflns_used Value .... Please Do !
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value ..... Please Do !
PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value ..... Please Do !
PLAT201_ALERT_2_A Isotropic non-H Atoms in Main Residue(s) ..... 14 Report

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Alert level B

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Ni2B --N3B . 10.3 s.u.

Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5765
WEIGH01_ALERT_1_C Extra text has been found in the
_refine_ls_weighting_scheme field. This should be in the
_refine_ls_weighting_details field.
Weighting scheme given as calc w=1/[\s^2^(Fo^2^)+(0.0416P)^2^+0.0000
Weighting scheme identified as calc
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.10 Check
PLAT155_ALERT_4_C The Triclinic Unitcell is NOT Reduced ..... Please Do !
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ni1A --O1A . 5.3 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ni1A --N3A . 5.4 s.u.
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of O7 Check

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Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C15.25 H21 Cl1 N3 Ni1 O6.25
Atom count from the _atom_site data: C15.25 H20.25 Cl1 N3 Ni1 O6.25
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C15.25 H21 Cl N3 Ni O6.25
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	61.00	61.00	0.00
H	84.00	81.00	3.00
Cl	4.00	4.00	0.00
N	12.00	12.00	0.00
Ni	4.00	4.00	0.00
O	25.00	25.00	0.00

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 8 Report
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 3 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.25 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) Cl2 --O9 . 15.0 s.u.
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of Cl1 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2 Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2' Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O8 Constrained at 0.6 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of O9       Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O10      Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O8'      Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O9'      Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O10'     Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O11      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11      Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3)        80% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ......                  5. Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....     C15A Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl2'   ..O11            2.96 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O10    ..C12A           3.01 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O11    ..C16            2.61 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O8'    ..C16            2.68 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C16    ..C16            1.34 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          6 Note
PLAT721_ALERT_1_G Bond    Calc     0.91000, Rep     0.84000 Dev...       0.07 Ang.
             O11    -H11           1.555   1.555 .............     #  102 Check
PLAT722_ALERT_1_G Angle   Calc      113.00, Rep      109.50 Dev...       3.50 Degree
             C16    -O11    -H11        1.555   1.555   1.555     #  180 Check
PLAT725_ALERT_2_G D-H     Calc     0.91000, Rep     0.84000 Dev...       0.07 Ang.
             O11    -H11           1.555   1.555 .............     #  103 Check
PLAT726_ALERT_2_G H...A   Calc     2.88000, Rep     2.02000 Dev...       0.86 Ang.
             H11    -O2B           1.555   1.555 .............     #  103 Check
PLAT728_ALERT_1_G D-H..A  Calc       65.00, Rep      129.00 Dev...      64.00 Degree
             O11    -H11    -O2B        1.555   1.555   1.555     #  181 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      179 Check
             CL2' -O7   -CL2     1.555   1.555   1.555             29.90 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
             Cl O4
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found     Please Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        12 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2016 Note
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   5 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  41 ALERT level G = General information/check it is not something unexpected

  13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
  23 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. 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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_THETM01_ad56
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.590
RESPONSE: ...
;
_vrf_WEIGH01_ad56
;
PROBLEM: Extra text has been found in the
RESPONSE: ...
;
_vrf_PLAT029_ad56
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .      0.927 Why?
RESPONSE: ...
;
_vrf_PLAT183_ad56
;
PROBLEM: Missing _cell_measurement_reflns_used Value ....     Please Do !
RESPONSE: ...
;
_vrf_PLAT184_ad56
;
PROBLEM: Missing _cell_measurement_theta_min Value ......     Please Do !
RESPONSE: ...
;
_vrf_PLAT185_ad56
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;
PROBLEM: Missing _cell_measurement_theta_max Value ......     Please Do !
RESPONSE: ...
;
_vrf_PLAT201_ad56
;
PROBLEM: Isotropic non-H Atoms in Main Residue(s) .......         14 Report
RESPONSE: ...
;
_vrf_PLAT041_ad56
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT043_ad56
;
PROBLEM: Calculated and Reported Mol. Weight Differ by ..       3.10 Check
RESPONSE: ...
;
_vrf_PLAT155_ad56
;
PROBLEM: The Triclinic Unitcell is NOT Reduced ..........     Please Do !
RESPONSE: ...
;
_vrf_PLAT232_ad56
;
PROBLEM: Hirshfeld Test Diff (M-X) Ni1A   --O1A     .        5.3 s.u.
RESPONSE: ...
;
_vrf_PLAT243_ad56
;
PROBLEM: High   'Solvent' Ueq as Compared to Neighbors of       O7 Check
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 13/08/2017; check.def file version of 12/12/2017

Datablock ad56 - ellipsoid plot