checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: asb101

Bond precision: C-C = 0.0032 A Wavelength=0.71073

Cell: **a=9.3786(5) b=18.1064(9) c=17.4684(9)**
alpha=90 beta=93.4637(6) gamma=90
Temperature: 153 K

	Calculated	Reported
Volume	2960.9(3)	2960.9(3)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C29 H37 Cl2 N5 Ni O2	?
Sum formula	C29 H37 Cl2 N5 Ni O2	C29 H37 Cl2 N5 Ni O2
Mr	617.23	617.25
Dx,g cm-3	1.385	1.385
Z	4	4
Mu (mm-1)	0.871	0.871
F000	1296.0	1296.0
F000'	1298.89	
h,k,lmax	12,23,22	12,23,22
Nref	6519	6508
Tmin,Tmax	0.818,0.878	0.825,0.881
Tmin'	0.818	

Correction method= MULTI-SCAN

Data completeness= 0.998 Theta(max)= 27.100

R(reflections)= 0.0382(5858) wR2(reflections)= 0.1057(6508)

S = 1.053 Npar= 467

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

PLAT222_ALERT_3_A Large Non-Solvent H Ueq(max)/Ueq(min) ... 5.88 Ratio

---

Alert level B

PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density 4.34
PLAT391_ALERT_3_B Deviating Methyl C10 H-C-H Bond Angle ..... 99.00 Deg.

Alert level C

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 2.69 Ratio
PLAT351_ALERT_3_C Long C-H Bond (0.96A) C10 - H10C ... 1.13 Ang.
PLAT390_ALERT_3_C Deviating Methyl C11 X-C-H Bond Angle ..... 117.10 Deg.

Alert level G

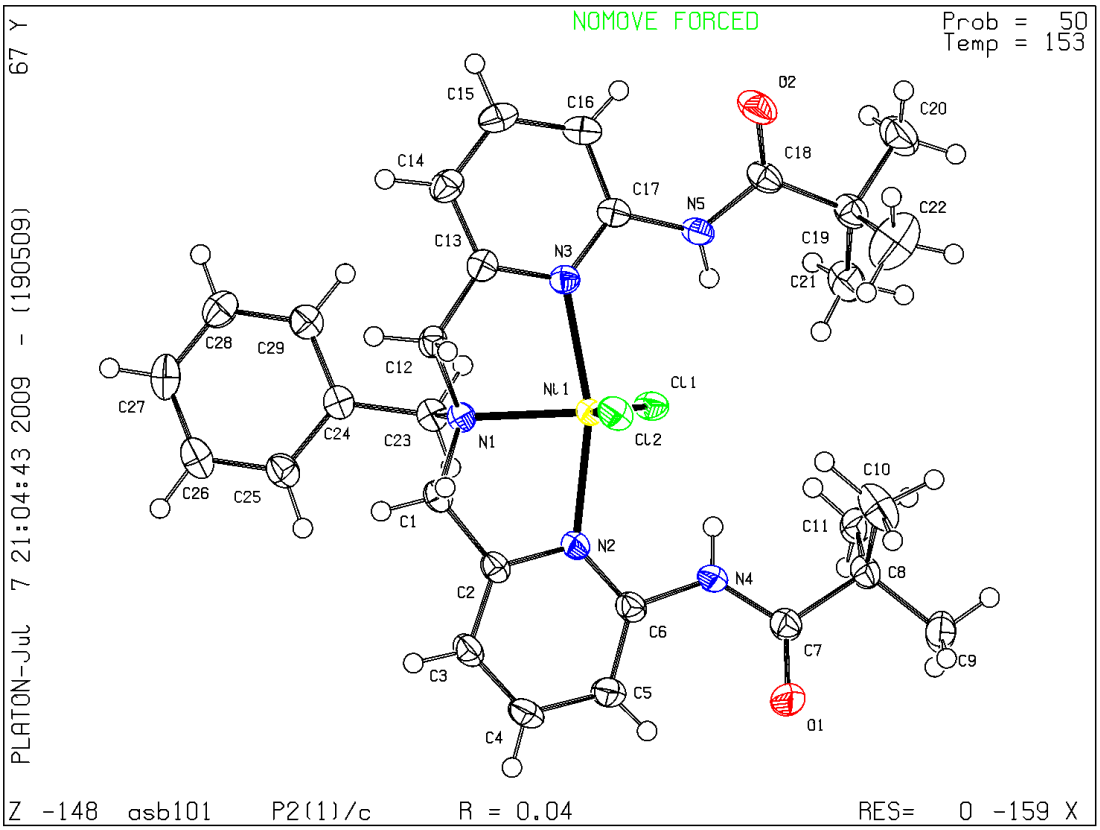
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 26

1 **ALERT level A** = In general: serious problem
2 **ALERT level B** = Potentially serious problem
3 **ALERT level C** = Check and explain
1 **ALERT level G** = General alerts; check

0 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
4 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 19/05/2009; check.def file version of 13/05/2009

Datablock asb101 - ellipsoid plot



checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: asb124

Bond precision: C-C = 0.0040 A Wavelength=0.71073

Cell: **a=13.452(2) b=14.834(3) c=17.896(3)**
alpha=90 beta=102.073(2) gamma=90
Temperature: 153 K

	Calculated	Reported
Volume	3492.1(11)	3492.4(10)
Space group	P c	Pc
Hall group	P -2yc	?
Moiety formula	C33 H43 N5 Ni O6, C2 H3 N	?
Sum formula	C35 H46 N6 Ni O6	C35 H46 N6 Ni O6
Mr	705.47	705.49
Dx,g cm-3	1.342	1.342
Z	4	4
Mu (mm-1)	0.609	0.609
F000	1496.0	1496.0
F000'	1497.91	
h,k,lmax	17,19,22	17,19,22
Nref	7718[15417]	15208
Tmin,Tmax	0.848,0.958	0.853,0.961
Tmin'	0.848	

Correction method= MULTI-SCAN

Data completeness= 1.97/0.99 Theta(max)= 27.100

R(reflections)= 0.0363(12167) wR2(reflections)= 0.0807(15208)

S = 1.004 Npar= 900

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
PLAT222_ALERT_3_A Large Non-Solvent H Ueq(max)/Ueq(min) ... 5.08 Ratio

---

Alert level C
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.372

```
          From the CIF: _refine_ls_abs_structure_Flack_su    0.007
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Ni2    --  O9      ..       6.63 su
PLAT245_ALERT_2_C U(iso) H5      Smaller than U(eq) N5      by ...       0.01 AngSq
PLAT352_ALERT_3_C Short   N-H Bond (0.87A)   N9     -   H9     ...       0.74 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          2
             C33 H43 N5 Ni O6
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          3
             C2 H3 N
```

Alert level G

```
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
           correct. If it is not, please give the correct count in the
           _publ_section_exptl_refinement section of the submitted CIF.
          From the CIF: _diffrn_reflns_theta_max           27.10
          From the CIF: _reflns_number_total              15208
          Count of symmetry unique reflns         7718
          Completeness (_total/calc)            197.05%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured      7490
          Fraction of Friedel pairs measured     0.970
          Are heavy atom types Z>Si present        yes
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......          2
PLAT033_ALERT_4_G Flack x Parameter Value Deviates from Zero .....       0.37
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        144
            O5  -NI1 -C30 -C31    80.00  5.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        145
            N1  -NI1 -C30 -C31  -102.00  5.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        146
            O3  -NI1 -C30 -C31    80.00  5.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        147
            N2  -NI1 -C30 -C31   175.00  5.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        148
            N3  -NI1 -C30 -C31   -19.00  5.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        149
            O4  -NI1 -C30 -C31  -103.00  5.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        295
            O11 -NI2 -C63 -C64   107.00  7.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        296
            N6  -NI2 -C63 -C64   -67.00  7.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        297
            O10 -NI2 -C63 -C64   -66.00  7.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        298
            N7  -NI2 -C63 -C64  -151.00  7.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        299
            N8  -NI2 -C63 -C64    14.00  7.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        300
            O9  -NI2 -C63 -C64   115.00  7.00   1.555   1.555   1.555   1.555
```

```
   1 ALERT level A = In general: serious problem
   0 ALERT level B = Potentially serious problem
   6 ALERT level C = Check and explain
  15 ALERT level G = General alerts; check

   0 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
   3 ALERT type 3 Indicator that the structure quality may be low
  17 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Publication of your CIF in IUCr journals

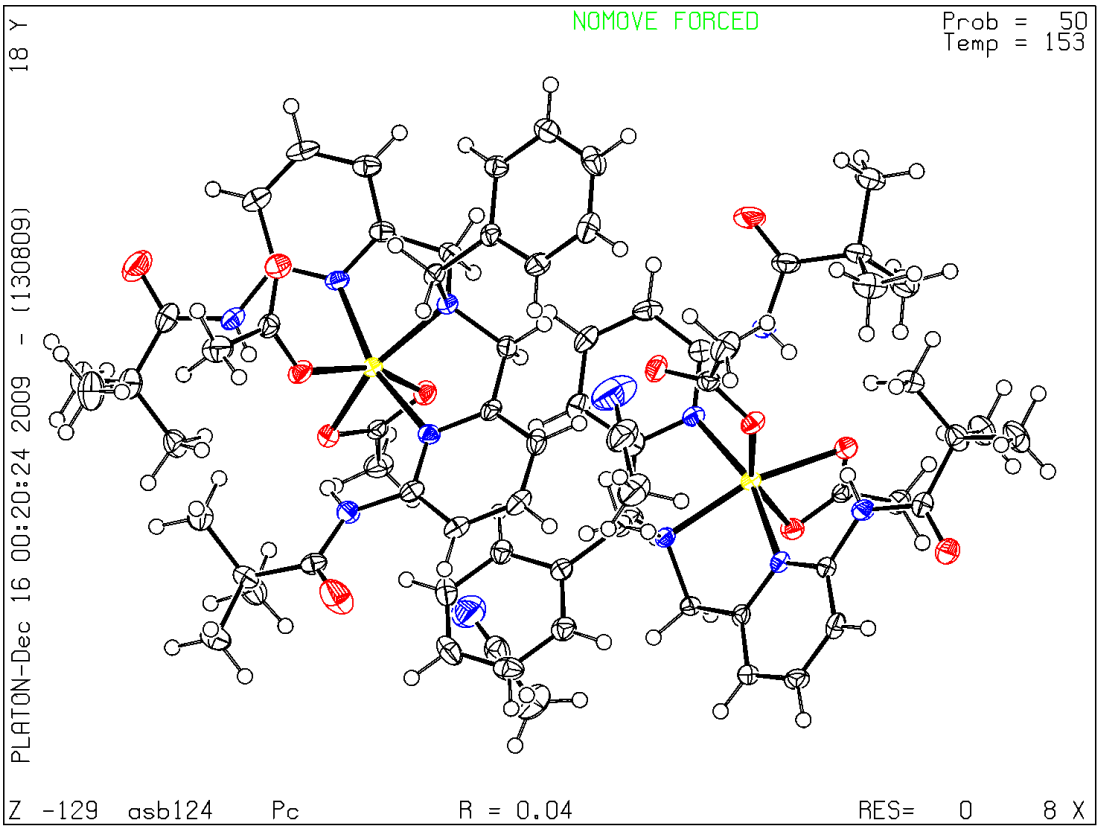
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 13/08/2009; check.def file version of 12/08/2009

Datablock asb124 - ellipsoid plot



checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: asb130

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=9.8123(5) b=11.8641(6) c=13.4619(7)
alpha=82.8894(7) beta=82.2732(7) gamma=88.6757(7)
Temperature: 98 K

	Calculated	Reported
Volume	1540.95(14)	1540.95(14)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C31 H39 N5 Ni O3, C2 H4	?
Sum formula	C33 H43 N5 Ni O3	C33 H43 N5 Ni O3
Mr	616.41	616.43
Dx,g cm-3	1.329	1.329
Z	2	2
Mu (mm-1)	0.671	0.671
F000	656.0	656.0
F000'	656.89	
h,k,lmax	12,15,17	12,15,17
Nref	6802	6753
Tmin,Tmax	0.901,0.916	0.866,0.918
Tmin'	0.863	

Correction method= MULTI-SCAN

Data completeness= 0.993 Theta(max)= 27.100

R(reflections)= 0.0399(5622) wR2(reflections)= 0.1032(6753)

S = 1.028 Npar= 381

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

PLAT432_ALERT_2_A Short Inter X...Y Contact	O3	..	C31	..	2.33	Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact	O3	..	C32	..	2.35	Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact	O3	..	C32A	..	2.37	Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact	O3	..	C31A	..	2.38	Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact	C31A	..	C30	..	1.32	Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact	C31A	..	C33A	..	2.39	Ang.

```
PLAT432_ALERT_2_A Short Inter X...Y Contact  C32    ..  C33A    ..       1.44 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact  C32    ..  C30     ..       2.32 Ang.
```

Alert level B

```
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .......          5
PLAT413_ALERT_2_B Short Inter XH3 .. XHn     H23A   ..  H11E    ..       2.07 Ang.
```

Alert level C

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.18
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          2
PLAT222_ALERT_3_C Large Non-Solvent    H     Ueq(max)/Ueq(min) ...       3.24 Ratio
PLAT195_ALERT_1_C Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_C Missing _cell_measurement_theta_min   datum ....          ?
```

Alert level G

```
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................      11.00 Perc.
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal  (x 10000)         70 Deg.
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................      50.00 Perc.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          3
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      12.80 Deg.
              C30A -O3   -C30     1.555   1.555   1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      23.30 Deg.
              C33A -O3   -C33     1.555   1.555   1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      38.50 Deg.
              C10A -C8   -C10     1.555   1.555   1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      34.10 Deg.
              C9   -C8   -C9A     1.555   1.555   1.555
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          !
```

```
   8 ALERT level A = In general: serious problem
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   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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   1 ALERT type 5 Informative message, check
```

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

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PLATON version of 13/08/2009; check.def file version of 12/08/2009

Datablock asb130 - ellipsoid plot