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: d488

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Bond precision:   C-C = 0.0068 A            Wavelength=1.54184

Cell:           a=19.2947(6)     b=15.1426(6)         c=20.4291(6)
                alpha=90         beta=103.384(3)      gamma=90
Temperature:    293 K

                Calculated                 Reported
Volume          5806.7(3)                  5806.7(3)
Space group     C 2/c                      C 1 2/c 1
Hall group      -C 2yc                     -C 2yc
                C44 H54 N4 Ni3 O16, 2(H2   C44 H54 N4 Ni3 O16, 2(H2
Moiety formula  O) [+ solvent]             O)
                C44 H58 N4 Ni3 O18 [+
Sum formula     solvent]                   C44 H58 N4 Ni3 O18
Mr              1107.01                    1107.07
Dx,g cm-3       1.266                      1.266
Z               4                          0
Mu (mm-1)       1.683                      1.683
F000            2312.0                     2312.0
F000'           2282.78
h,k,lmax        23,18,24                   23,18,24
Nref            5465                       5377
Tmin,Tmax       0.769,0.817                0.958,1.000
Tmin'           0.714


Correction method= # Reported T Limits: Tmin=0.958 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.984          Theta(max)= 69.648

R(reflections)= 0.0557( 4045)     wR2(reflections)= 0.1768( 5377)

S = 1.090                    Npar= 338
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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   O9   --H9C   Please Check

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🟡 Alert level C
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.60 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C   Ueq(max)/Ueq(min) Range   5.5 Ratio
PLAT222_ALERT_3_C Non-Solv. Resd 1   H   Uiso(max)/Uiso(min) Range   6.1 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for   O3   --C9   .   5.7 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21   --C22   0.24 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C9 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C22 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   O6 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 ....   0.00676 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C8   - C9   .   1.34 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H8B   ..H9B   1.96 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn   H20A   ..H21A   1.86 Ang.
PLAT417_ALERT_2_C Short Inter D-H..H-D   H6A   ..H9D   2.10 Ang.

⚪ Alert level G
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   11 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   3 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   1 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large   0.11 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   5 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records   4 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records   2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records   2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records   2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K)   293 Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C21'   --C22   .   8.6 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of C21   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21'   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6A   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6B   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21A   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21B   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21C   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21D   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22A   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22B   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22C   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22D   Constrained at   0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   3% Note
PLAT395_ALERT_2_G Deviating X-O-Y   Angle From 120 for O2   112.3 Degree
PLAT395_ALERT_2_G Deviating X-O-Y   Angle From 120 for O3   109.6 Degree
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure   269 A**3
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   35 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
  14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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   29 ALERT level G = General information/check it is not something unexpected

    2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   18 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
   19 ALERT type 4 Improvement, methodology, query or suggestion
    1 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

NOMOVE FORCED

Prob = 50
Temp = 293

33 Y

PLATON-Mar 17 05:03:46 2018 - (70316)

Z -106 d488 C 1 2/c 1 R = 0.06 RES= 0 -39 X