checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

```
Bond precision:    C-C = 0.0300 A            Wavelength=0.71073

Cell:              a=18.4946(9)     b=18.4946(9)      c=18.1930(9)
                   alpha=90         beta=90           gamma=90
Temperature:       170 K

                   Calculated                Reported
Volume             6222.9(7)                 6222.9(7)
Space group        P 4 n c                   P 4 n c
Hall group         P 4 -2n                   P 4 -2n
Moiety formula     C40 H48 N32 Ni4 S8, O     C40 H48 N32 Ni4 O S8
Sum formula        C40 H48 N32 Ni4 O S8      C40 H48 N32 Ni4 O S8
Mr                 1484.34                   1484.42
Dx,g cm-3          0.792                     0.792
Z                  2                         2
Mu (mm-1)          0.761                     0.761
F000               1520.0                    1520.0
F000'              1524.91
h,k,lmax           21,21,21                  21,21,21
Nref               5397[ 2795]               5129
Tmin,Tmax          0.859,0.927               0.610,0.856
Tmin'              0.859

Correction method= # Reported T Limits: Tmin=0.610 Tmax=0.856
AbsCorr = NUMERICAL

Data completeness= 1.84/0.95      Theta(max)= 24.841

R(reflections)= 0.1231( 3043)     wR2(reflections)= 0.3610( 5129)

S = 1.216                   Npar= 193
```

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.

[IMAGE] **Alert level A**
PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure   ! Info

[IMAGE] **Alert level B**
RINTA01_ALERT_3_B The value of Rint is greater than 0.18
             Rint given   0.183
PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ....   0.183 Report
PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ....   0.7922 Check
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ....   0.36 Report
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O1 Check
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ....   0.03 Ang.
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....   2 Check

[IMAGE] **Alert level C**
STRVA01_ALERT_4_C   Flack test results are ambiguous.
             From the CIF: _refine_ls_abs_structure_Flack   0.350
             From the CIF: _refine_ls_abs_structure_Flack_su   0.090
PLAT082_ALERT_2_C High R1 Value ....   0.12 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.76 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ....   1 Check
PLAT415_ALERT_2_C Short Inter D-H..H-X   H4B   ..H5'C   2.13 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor   N4'   --H4'B   Please Check
PLAT420_ALERT_2_C D-H Without Acceptor   N4   --H4B   Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.591   45 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .   2 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.96A   From C5'   1.74 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 3.15A   From O1   1.74 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.78A   From N4'   1.66 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.91A   From N4   1.55 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.60A   From O1   1.09 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.   0 Info

[IMAGE] **Alert level G**
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   4 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large   0.20 Report
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd 2   0.25 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C5 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C5' Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   5 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).   2 Note

   1 **ALERT level A** = Most likely a serious problem - resolve or explain
   7 **ALERT level B** = A potentially serious problem, consider carefully
  15 **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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  14 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check

checkCIF publication errors

[IMAGE] **Alert level A**
```
PUBL004_ALERT_1_A  The contact author's name and address are missing,
            _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
            _publ_contact_author_phone are all missing.
            At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
            e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
```

[IMAGE] **Alert level G**
```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

```
   7 ALERT level A = Data missing that is essential or data in wrong format
   1 ALERT level G = General alerts. Data that may be required is missing
```

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

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_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
```

```
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PLAT602_I
;
PROBLEM: VERY LARGE Solvent Accessible VOID(S) in Structure        ! Info
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 30/01/2018; check.def file version of 30/01/2018

Datablock I - ellipsoid plot

NOMOVE FORCED

Prob = 50
Temp = 170

PLATON-Apr 20 11:36:31 2018 - (70316)

Z -67   I   P 4 n c   R = 0.12   RES=   0   0 X