## 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 = 0.0101 A Wavelength=0.71073 Cell: a=8.136(3) b=12.552(4) c=14.333(5) alpha=92.373(4) beta=98.971(4) gamma=108.891(4) Temperature: 291 K Calculated Reported Volume 1361.3(8) 1361.3(8) P -1 Space group P -1 Hall group -P 1 -P 1 C17 H13 N2, C8 N4 Ni S4 [+ C17 H13 N2, C8 N4 Ni S4 Moiety formula solvent] C25 H13 N6 Ni S4 [+ Sum formula C25 H13 N6 Ni S4 solvent] 584.34 584.36 Mr 1.426 1.426 Dx,q cm-3 Ζ 2 2 Mu (mm-1) 1.045 1.045 F000 594.0 594.0 F000′ 595.79 h,k,lmax 9,14,17 9,14,17 4799 Nref 4710 Tmin,Tmax 0.839,0.891 0.846,0.891 Tmin′ 0.837 Correction method= # Reported T Limits: Tmin=0.846 Tmax=0.891 AbsCorr = MULTI-SCAN Data completeness= 0.981 Theta(max) = 25.029R(reflections) = 0.0761( 3409) wR2(reflections) = 0.2315( 4710) S = 1.079Npar= 326

# 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 C

PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full	!	Check
PLAT234_ALERT_4_C Large Hirshfeld Difference C19C20 .	0.16	Ang.
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds	0.01009	Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	2.972	Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595	70	Report

#### Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.12	Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal(Note)	0.004	Degree
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure	124	A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1 (III) .	3.02	Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed	!	Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still	39%	Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT931_ALERT_5_G CIFcalcFCF Twin Law (010) Est.d BASF	0.15	Check
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities	Please	Check
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by	1	Check

```
0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
13 ALERT level G = General information/check it is not something unexpected
4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check
```

### checkCIF publication errors

#### 🔩 Alert level A

```
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.
```

#### Alert level G

PUBL017\_ALERT\_1\_G The \_publ\_section\_references section is missing or empty. 5 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_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: ...
# 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 22/12/2019; check.def file version of 13/12/2019

Datablock I - ellipsoid plot

