

# 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

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Bond precision:	C-C = 0.0137 Å	Wavelength=0.71073
Cell:	a=7.9700(14)	b=12.362(2)      c=14.157(3)
	alpha=90.764(5)	beta=99.113(5)      gamma=107.676(5)
Temperature:	85 K	
	Calculated	Reported
Volume	1309.4(4)	1309.4(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C17 H13 N2, C8 N4 Ni S4 [+ solvent]	C17 H13 N2, C8 N4 Ni S4
Sum formula	C25 H13 N6 Ni S4 [+ solvent]	C25 H13 N6 Ni S4
Mr	584.34	584.36
Dx, g cm <sup>-3</sup>	1.482	1.482
Z	2	2
Mu (mm <sup>-1</sup> )	1.086	1.086
F000	594.0	594.0
F000'	595.79	
h,k,lmax	9,14,16	9,14,16
Nref	4618	4358
Tmin,Tmax	0.791,0.878	0.798,0.871
Tmin'	0.779	
Correction method= # Reported T Limits: Tmin=0.798 Tmax=0.871		
AbsCorr = MULTI-SCAN		
Data completeness=	0.944	Theta(max)= 25.000
R(reflections)=	0.0977( 3781)	wR2(reflections)= 0.2331( 4358)
S =	1.219	Npar= 325

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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.

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### Alert level B

PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low .	0.944	Why?
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L=	0.595	259 Report

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### Alert level C

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....	2.3	Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds .....	0.01374	Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # C17 H13 N2	1	Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....	9.808	Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....	2.966	Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.00A From N4	0.80	eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.	0	Info

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### Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...	7	Report
PLAT014_ALERT_1_G N.O.K. _shelx_fab_checksum Found in CIF .....		Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	25.28	Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal..(Note)	0.005	Degree
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure	110	A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1 (III) .	3.01	Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....	30	Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE 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	73%	Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....	3	Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...	2	Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
2 **ALERT level B** = A potentially serious problem, consider carefully  
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
14 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
6 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  
4 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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## checkCIF publication errors

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### 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.

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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

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## 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.

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**PLATON version of 22/12/2019; check.def file version of 13/12/2019**

Datablock I - ellipsoid plot

