

# 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 = 0.0475 A	Wavelength=0.71073	
Cell:	a=20.065(2)	b=20.065(2)	c=19.1367(18)
	alpha=90	beta=90	gamma=90
Temperature:	170 K		
	Calculated	Reported	
Volume	7704.5(17)	7704.5(17)	
Space group	I 4 2 2	I 4 2 2	
Hall group	I 4 2	I 4 2	
Moiety formula	C48 H64 N32 Ni4 S8, O	C48 H64 N32 Ni4 O S8	
Sum formula	C48 H64 N32 Ni4 O S8	C48 H64 N32 Ni4 O S8	
Mr	1596.55	1596.63	
Dx,g cm-3	0.688	0.688	
Z	2	2	
Mu (mm-1)	0.617	0.617	
F000	1648.0	1648.0	
F000'	1652.94		
h,k,lmax	23,23,22	23,23,22	
Nref	3299[ 1883]	3261	
Tmin,Tmax	0.831,0.831	0.441,0.688	
Tmin'	0.831		

Correction method= # Reported T Limits: Tmin=0.441 Tmax=0.688  
AbsCorr = NUMERICAL

Data completeness= 1.73/0.99      Theta(max)= 24.689

R(reflections)= 0.1743( 794)      wR2(reflections)= 0.4928( 3261)

S = 1.102      Npar= 72

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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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[IMAGE] **Alert level A**

RINTA01\_ALERT\_3\_A The value of Rint is greater than 0.25  
Rint given 0.315  
PLAT020\_ALERT\_3\_A The Value of Rint is Greater Than 0.12 ..... 0.315 Report  
PLAT026\_ALERT\_3\_A Ratio Observed / Unique Reflections (too) Low .. 24% Check  
PLAT084\_ALERT\_3\_A High wR2 Value (i.e. > 0.25) ..... 0.49 Report  
PLAT234\_ALERT\_4\_A Large Hirshfeld Difference N3 --C4 0.32 Ang.  
PLAT602\_ALERT\_2\_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

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[IMAGE] **Alert level B**

PLAT049\_ALERT\_1\_B Calculated Density Less Than 1.0 gcm-3 ..... 0.6882 Check  
PLAT082\_ALERT\_2\_B High R1 Value ..... 0.17 Report  
PLAT241\_ALERT\_2\_B High 'MainMol' Ueq as Compared to Neighbors of C3 Check  
PLAT306\_ALERT\_2\_B Isolated Oxygen Atom (H-atoms Missing ?) ..... 01 Check  
PLAT341\_ALERT\_3\_B Low Bond Precision on C-C Bonds ..... 0.0475 Ang.

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[IMAGE] **Alert level C**

THETM01\_ALERT\_3\_C The value of sine(theta\_max)/wavelength is less than 0.590  
Calculated sin(theta\_max)/wavelength = 0.5877  
PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 2.17 Report  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of S1 Check  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C4 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of N2 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of N3 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C2 Check  
PLAT360\_ALERT\_2\_C Short C(sp3)-C(sp3) Bond C5 - C6 . 1.34 Ang.  
PLAT363\_ALERT\_2\_C Long C(sp3)-C(sp2) Bond C3 - C5 . 1.63 Ang.  
PLAT420\_ALERT\_2\_C D-H Without Acceptor N4 --H4A Please Check  
PLAT420\_ALERT\_2\_C D-H Without Acceptor N4 --H4B Please Check  
PLAT905\_ALERT\_3\_C Negative K value in the Analysis of Variance ... -4.862 Report  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.471 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.386 Check  
PLAT907\_ALERT\_2\_C Flack x > 0.5, Structure Needs to be Inverted? . 0.70 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.588 14 Report  
PLAT978\_ALERT\_2\_C Number C-C Bonds with Positive Residual Density. 0 Info

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[IMAGE] **Alert level G**

PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 8 Report  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 2 Report  
PLAT033\_ALERT\_4\_G Flack x Value Deviates > 3.0 \* sigma from Zero . 0.700 Note  
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  
PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 4 Report  
PLAT174\_ALERT\_4\_G The CIF-Embedded .res File Contains FLAT Records 1 Report  
PLAT177\_ALERT\_4\_G The CIF-Embedded .res File Contains DELU Records 4 Report  
PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 4 Report  
PLAT186\_ALERT\_4\_G The CIF-Embedded .res File Contains ISOR Records 4 Report  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... Resd 2 0.13 Check  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 1 Note  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 85 Note  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note  
PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 2 Note

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6 **ALERT level A** = Most likely a serious problem - resolve or explain

5 **ALERT level B** = A potentially serious problem, consider carefully

17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
19 ALERT type 2 Indicator that the structure model may be wrong or deficient  
12 ALERT type 3 Indicator that the structure quality may be low  
9 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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### [IMAGE] 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.  
PUBL012\_ALERT\_1\_A \_publ\_section\_abstract is missing.  
Abstract of paper in English.

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### [IMAGE] Alert level G

PUBL017\_ALERT\_1\_G The \_publ\_section\_references section is missing or  
empty.

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3 **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
```

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RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_RINTA01_I
;
PROBLEM: The value of Rint is greater than 0.25
RESPONSE: ...
;
_vrf_PLAT020_I
;
PROBLEM: The Value of Rint is Greater Than 0.12 ..... 0.315 Report
RESPONSE: ...
;
_vrf_PLAT026_I
;
PROBLEM: Ratio Observed / Unique Reflections (too) Low .. 24% Check
RESPONSE: ...
;
_vrf_PLAT084_I
;
PROBLEM: High wR2 Value (i.e. > 0.25) ..... 0.49 Report
RESPONSE: ...
;
_vrf_PLAT234_I
;
PROBLEM: Large Hirshfeld Difference N3 --C4 0.32 Ang.
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.

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

