

## checkCIF (full publication check) running

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Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait .....

## checkCIF/PLATON (full publication check)

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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.  
Please wait while processing ....

[CIF dictionary](#)  
[Interpreting this report](#)

[Structure factor report](#)

## Datablock: I

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Bond precision:	C-C = 0.0162 A	Wavelength=0.71073
Cell:	a=19.422(2)      b=22.654(3)      c=25.321(3)	
	alpha=115.783(4)    beta=92.992(5)    gamma=106.118(5)	
Temperature:	150 K	
	Calculated	Reported
Volume	9443(2)	9443(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C133 H87 C15 I2 N9 Ni12 O35, I [+ solvent]	C133 H101 C15 I2 N9 Ni12 O35, I
Sum formula	C133 H87 C15 I3 N9 Ni12 O35 [+ solvent]	C133 H101 C15 I3 N9 Ni12 O35
Mr	3633.35	3647.69
Dx, g cm-3	1.278	1.283
Z	2	2
Mu (mm-1)	1.786	1.786
F000	3616.0	3644.0
F000'	3624.08	
h,k,lmax	23,26,30	23,26,30
Nref	33355	32481
Tmin,Tmax	0.807,0.931	0.675,0.931
Tmin'	0.675	
Correction method=	# Reported T Limits: Tmin=0.675 Tmax=0.931	
AbsCorr =	MULTI-SCAN	
Data completeness=	0.974	Theta(max)= 25.027
R(reflections)=	0.0872( 23114)	wR2(reflections)= 0.2361( 32481)
S =	1.040	Npar= 1787

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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 A

[PLAT910\\_ALERT\\_3\\_A](#) Missing # of FCF Reflection(s) Below Theta(Min). 114 Note

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### Alert level B

[PLAT220\\_ALERT\\_2\\_B](#) Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 7.0 Ratio

**And 2 other PLAT220 Alerts**

[More ...](#)

[PLAT242\\_ALERT\\_2\\_B](#) Low 'MainMol' Ueq as Compared to Neighbors of Ni9 Check

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### Alert level C

[PLAT029\\_ALERT\\_3\\_C](#) \_diffn\_measured\_fraction\_theta\_full value Low . 0.974 Why?

[PLAT213\\_ALERT\\_2\\_C](#) Atom C114 has ADP max/min Ratio ..... 3.2 prolat

[PLAT213\\_ALERT\\_2\\_C](#) Atom C116 has ADP max/min Ratio ..... 3.7 prolat

[PLAT222\\_ALERT\\_3\\_C](#) Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 5.9 Ratio

[PLAT230\\_ALERT\\_2\\_C](#) Hirshfeld Test Diff for O21 --C48 . 5.5 s.u.

**And 2 other PLAT230 Alerts**

[More ...](#)

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference C85 --C86 . 0.16 Ang.

**And 2 other PLAT234 Alerts**

[More ...](#)

[PLAT241\\_ALERT\\_2\\_C](#) High 'MainMol' Ueq as Compared to Neighbors of C45 Check

[PLAT241\\_ALERT\\_2\\_C](#) High 'MainMol' Ueq as Compared to Neighbors of C67 Check

[PLAT242\\_ALERT\\_2\\_C](#) Low 'MainMol' Ueq as Compared to Neighbors of Ni4 Check

**And 5 other PLAT242 Alerts**

[More ...](#)

[PLAT260\\_ALERT\\_2\\_C](#) Large Average Ueq of Residue Including I8 0.076 Check

[PLAT342\\_ALERT\\_3\\_C](#) Low Bond Precision on C-C Bonds ..... 0.0162 Ang.

[PLAT369\\_ALERT\\_2\\_C](#) Long C(sp2)-C(sp2) Bond C6 - C7 . 1.53 Ang.

[PLAT369\\_ALERT\\_2\\_C](#) Long C(sp2)-C(sp2) Bond C48 - C49 . 1.54 Ang.

[PLAT410\\_ALERT\\_2\\_C](#) Short Intra H...H Contact H4 ..H19 . 1.95 Ang.

x,y,z = 1\_555 Check

[PLAT911\\_ALERT\\_3\\_C](#) Missing FCF Refl Between Thmin & STh/L= 0.595 761 Report

[PLAT913\\_ALERT\\_3\\_C](#) Missing # of Very Strong Reflections in FCF .... 6 Note

[PLAT918\\_ALERT\\_3\\_C](#) Reflection(s) with I(obs) much Smaller I(calc) . 1 Check

[PLAT923\\_ALERT\\_1\\_C](#) S Values in the CIF and FCF Differ by ..... 0.012 Check

[PLAT934\\_ALERT\\_3\\_C](#) Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check

[PLAT973\\_ALERT\\_2\\_C](#) Check Calcd Positive Resid. Density on Ni6 1.30 eA-3

**And 6 other PLAT973 Alerts**

[More ...](#)

[PLAT977\\_ALERT\\_2\\_C](#) Check Negative Difference Density on H45 -0.34 eA-3

[PLAT978\\_ALERT\\_2\\_C](#) Number C-C Bonds with Positive Residual Density. 0 Info

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### Alert level G

[FORMU01\\_ALERT\\_2\\_G](#) There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and the formula from the \_atom\_site\* data.

Atom count from \_chemical\_formula\_sum: C133 H101 Cl5 I3 N9 Ni12 O35

Atom count from the \_atom\_site data: C133 H87 Cl5 I3 N9 Ni12 O35

[CELLZ01\\_ALERT\\_1\\_G](#) Difference between formula and atom\_site contents detected.

[CELLZ01\\_ALERT\\_1\\_G](#) WARNING: H atoms missing from atom site list. Is this intentional?

From the CIF: \_cell\_formula\_units\_Z 2

From the CIF: \_chemical\_formula\_sum C133 H101 Cl5 I3 N9 Ni12 O35

TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	266.00	266.00	0.00
H	202.00	174.00	28.00
Cl	10.00	10.00	0.00
I	6.00	6.00	0.00
N	18.00	18.00	0.00
Ni	24.00	24.00	0.00
O	70.00	70.00	0.00

PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 3 Report  
 PLAT041\_ALERT\_1\_G Calc. and Reported SumFormula Strings Differ Please Check  
 PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check  
 PLAT066\_ALERT\_1\_G Predicted and Reported Tmin&Tmax Range Identical ? Check  
 PLAT068\_ALERT\_1\_G Reported F000 Differs from Calcd (or Missing)... Please Check  
 PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report  
 PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 102.13 Why ?  
 PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 6 Report  
 PLAT186\_ALERT\_4\_G The CIF-Embedded .res File Contains ISOR Records 1 Report  
 PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) I1 --Ni1 . 12.3 s.u.

**And 13 other PLAT232 Alerts**

More ...

PLAT300\_ALERT\_4\_G Atom Site Occupancy of I1 Constrained at 0.55 Check

**And 13 other PLAT300 Alerts**

More ...

PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1 ) 3% Note  
 PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 100% Note  
 PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 3 ) 100% Note  
 PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... Resd 2 0.65 Check  
 PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... Resd 3 0.35 Check  
 PLAT432\_ALERT\_2\_G Short Inter X...Y Contact C100 ..C110 3.15 Ang.  
 1-x,1-y,-z = 2\_665 Check

PLAT606\_ALERT\_4\_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info  
 PLAT794\_ALERT\_5\_G Tentative Bond Valency for Ni5 (II) . 1.99 Info

**And 4 other PLAT794 Alerts**

More ...

PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 18 Note  
 PLAT869\_ALERT\_4\_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info  
 PLAT909\_ALERT\_3\_G Percentage of I>2sig(I) Data at Theta(Max) Still 45% Note

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

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

## checkCIF publication errors

### 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.

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## Alert level G

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

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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

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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_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
```

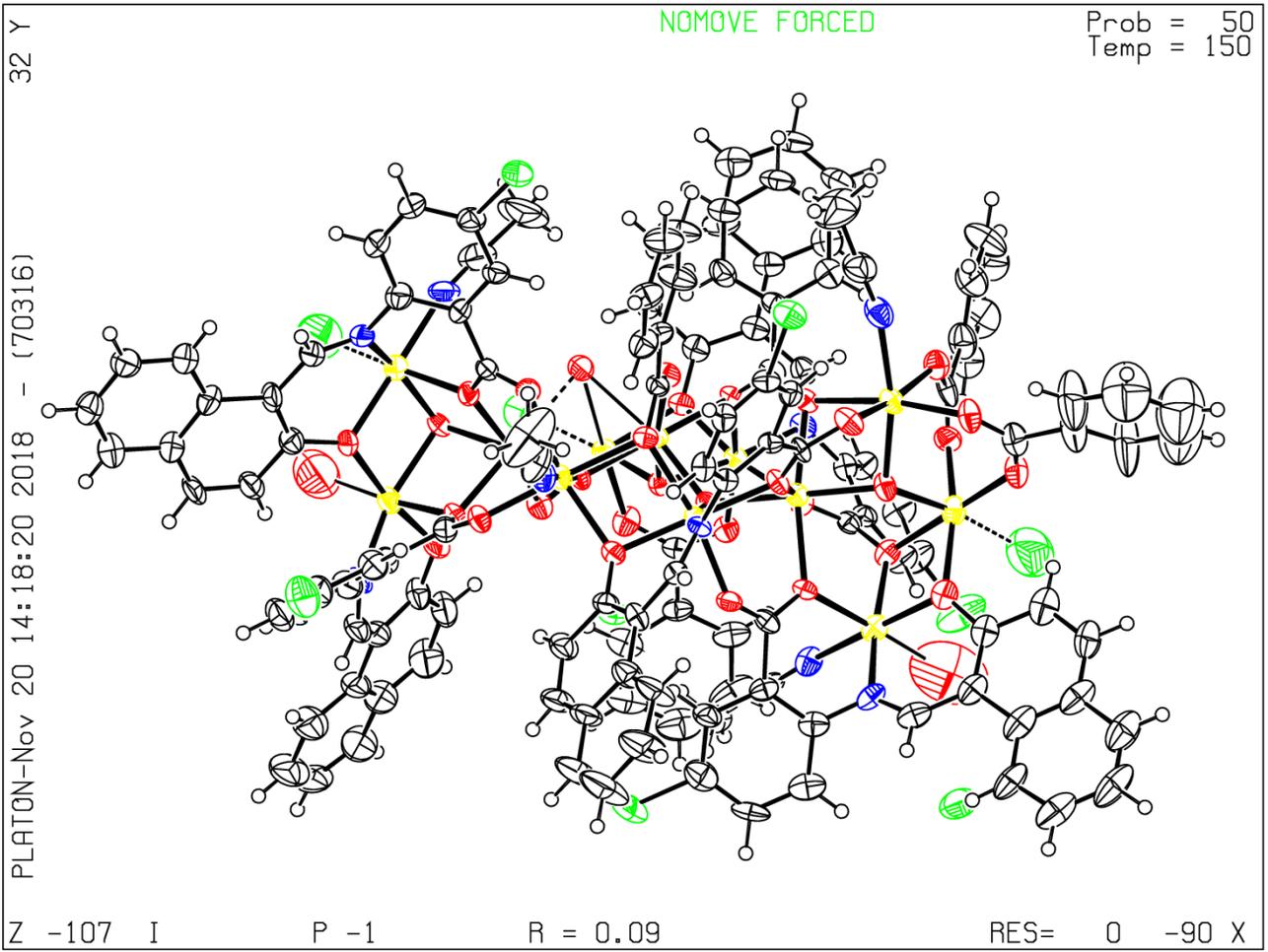
```
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PLAT910_I
;
PROBLEM: Missing # of FCF Reflection(s) Below Theta(Min).      114 Note
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 19/10/2018; check.def file version of 15/10/2018

## Datablock I - ellipsoid plot



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