

checkCIF/PLATON (full publication check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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](#)

Datablock: I

Bond precision:	C-C = 0.0053 A	Wavelength=0.71073	
Cell:	a=15.198(2)	b=16.132(2)	c=21.625(3)
	alpha=90	beta=97.749(2)	gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	5253.5(12)	5253.2(13)	
Space group	P 21/c	P2(1)/c	
Hall group	-P 2ybc	?	
Moiety formula	C40 H76 N8 Ni2 O4, 2(Cl O4), 3(H2 O)	?	
Sum formula	C40 H82 Cl2 N8 Ni2 O15	C40 H82 Cl2 N8 Ni2 O15	
Mr	1103.42	1103.46	
Dx,g cm-3	1.395	1.395	
Z	4	4	
Mu (mm-1)	0.887	0.887	
F000	2352.0	2352.0	
F000'	2356.84		
h,k,lmax	19,20,28	19,20,28	
Nref	12092	11857	
Tmin,Tmax	0.696,0.830	0.707,0.836	
Tmin'	0.682		
Correction method=	MULTI-SCAN		
Data completeness=	0.981	Theta(max)=	27.530
R(reflections)=	0.0507(7400)	wR2(reflections)=	0.1690(11857)
S =	1.040	Npar=	Npar = 634

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

[ABSTY02_ALERT_1_C](#) An _exptl_absorpt_correction_type has been given without

a literature citation. This should be contained in the

_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

[PLATO48_ALERT_1_C](#) MoietyFormula Not Given Please Do !

[PLAT125_ALERT_4_C](#) No '_symmetry_space_group_name_Hall' Given Please Do !

[PLAT230_ALERT_2_C](#) Hirshfeld Test Diff for O1 -- C17 .. 6.0 su

Alert level G

[PLAT002_ALERT_2_G](#) Number of Distance or Angle Restraints on AtSite 9 Note

[PLAT005_ALERT_5_G](#) No '_iucr_refine_instructions_details' in the CIF Please Do !

[PLAT007_ALERT_5_G](#) Number of Unrefined Donor-H Atoms 8 Why ?

[PLAT232_ALERT_2_G](#) Hirshfeld Test Diff (M-X) Ni1 -- O2 .. 8.9 su

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni2 -- O4 .. 7.9 su
 PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C11 Check
 PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C12 Check
 PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 13 Do !
 N5 -Ni2 -N7 -C33 -37.00 1.70 1.555 1.555 1.555 1.555

And 15 other PLAT710 Alerts

More ...

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 6 Note

PLAT793_ALERT_4_G The Model has Chirality at N1 R Verify

And 11 other PLAT793 Alerts

More ...

PLAT860_ALERT_3_G Number of Least-Squares Restraints 10 Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 4 ALERT type 2 Indicator that the structure model may be wrong or deficient
 1 ALERT type 3 Indicator that the structure quality may be low
 32 ALERT type 4 Improvement, methodology, query or suggestion
 2 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.

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.

```
# 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: ...

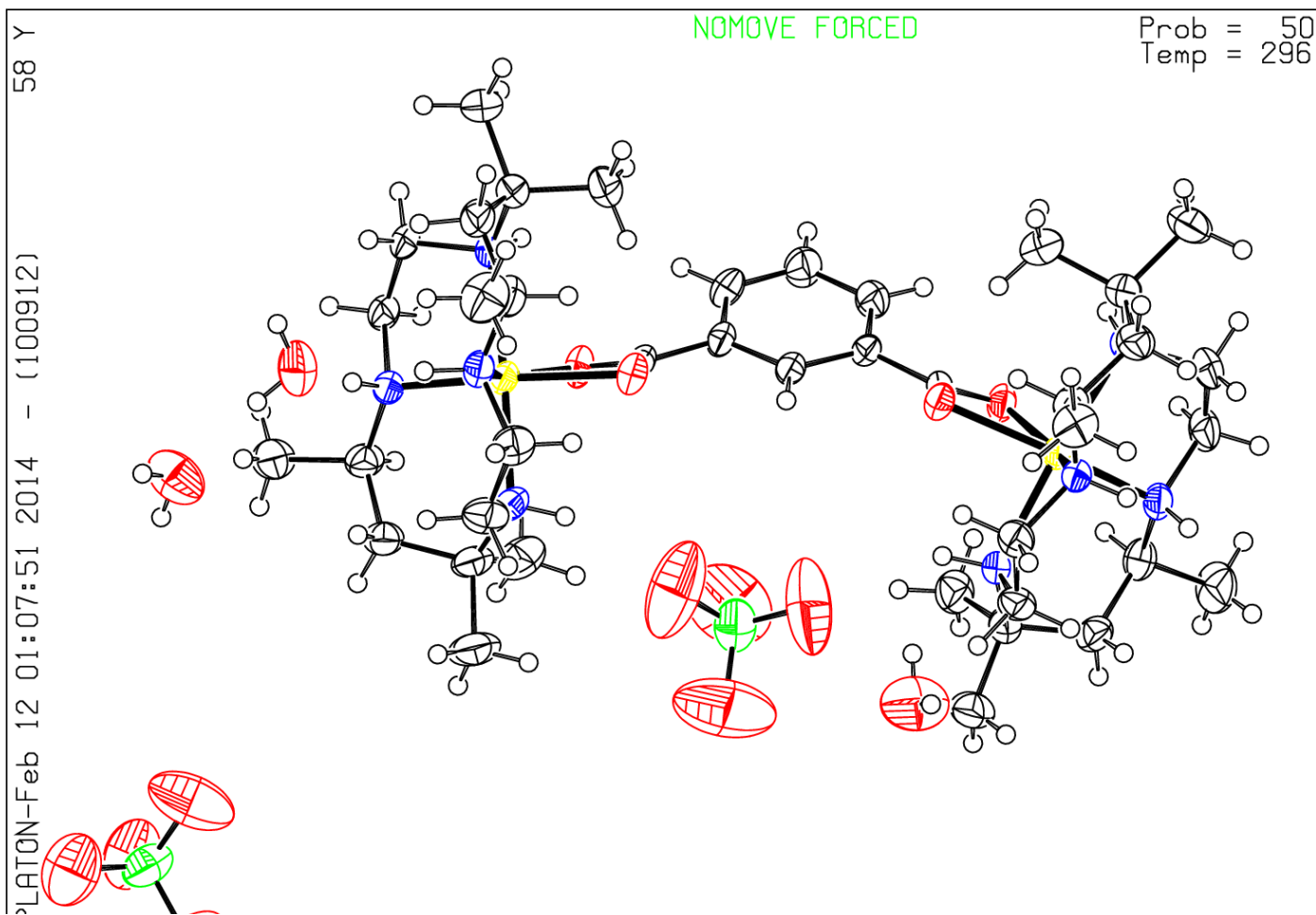
_vrf_PUBL012_GLOBAL

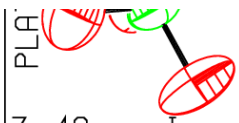
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...

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 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 05/02/2014; check.def file version of 05/02/2014

Datablock I - ellipsoid plot



Z 42

I

P2(1)/c

R = 0.05

RES= 0

48 X

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[Download CIF editor \(enCIFer\) from the CCDC](#)
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