

checkCIF (full publication check) running

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)

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

Bond precision:	C-C = 0.0162 Å	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 Cl5 I2 N9 Ni12 O35, I [+ solvent]	C133 H101 Cl5 I2 N9 Ni12 O35, I
Sum formula	C133 H87 Cl5 I3 N9 Ni12 O35 [+ solvent]	C133 H101 Cl5 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

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 A

PLAT910_ALERT_3_A Missing # of FCF Reflection(s) Below Theta(Min). 114 Note

🟡 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

🟢 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

🟢 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

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- 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.

● 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.

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

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;
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

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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 19/10/2018; check.def file version of 15/10/2018

Datablock I - ellipsoid plot

