

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

Bond precision: C-C = 0.0250 Å Wavelength=0.71073

Cell: a=18.8863(9) b=18.8863(9) c=18.4813(10)
 alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	6592.1(7)	6592.1(7)
Space group	I 4 2 2	I 4 2 2
Hall group	I 4 2	I 4 2
Moiety formula	C35.92 H35.76 N32 Ni4 S8, 4.08(C H3) [+ solvent]	C40 H48 N32 Ni4 S8
Sum formula	C40 H48 N32 Ni4 S8 [+ solvent]	C40 H48 N32 Ni4 S8
Mr	1468.34	1468.42
Dx, g cm ⁻³	0.740	0.740
Z	2	2
Mu (mm ⁻¹)	0.718	0.718
F000	1504.0	1504.0
F000'	1508.89	
h,k,lmax	23,23,23	23,23,23
Nref	3545[2014]	3526
Tmin,Tmax	0.866,0.931	0.459,0.855
Tmin'	0.866	

Correction method= # Reported T Limits: Tmin=0.459 Tmax=0.855
AbsCorr = NUMERICAL

Data completeness= 1.75/0.99 Theta(max)= 26.782

R(reflections)= 0.1191(1181) wR2(reflections)= 0.3937(3526)

S = 0.989 Npar= 97

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.

[IMAGE] **Alert level A**

RINTA01_ALERT_3_A The value of Rint is greater than 0.25
Rint given 0.273
PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 0.273 Report
PLAT417_ALERT_2_A Short Inter D-H..H-D H4A ..H4A 1.50 Ang.
PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Nil 2.06 eA-3

[IMAGE] **Alert level B**

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low .. 33% Check
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.39 Report
PLAT234_ALERT_4_B Large Hirshfeld Difference N4 --C4 0.26 Ang.
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.025 Ang.

[IMAGE] **Alert level C**

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.480
From the CIF: _refine_ls_abs_structure_Flack_su 0.110
PLAT082_ALERT_2_C High R1 Value 0.12 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 3.58 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 2.44 eA-3
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 1 Check
PLAT220_ALERT_2_C Non-Solvent Resd 1 N Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for N1 --C1_f . 5.4 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference N3 --C4 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1 --C2 0.18 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Nil Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C4 Check
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C1 - C2 . 1.54 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor N4 --H4B Please Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -1.155 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

[IMAGE] **Alert level G**

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 . 0.480 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
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 5% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 1 115.68 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 2 2.04 Check
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C2 - C3 . 1.53 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact N2 ..C5A 2.47 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact N3 ..C5A 2.28 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C3 ..C5A 1.92 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info
PLAT721_ALERT_1_G Bond Calc 0.97000, Rep 0.96000 Dev... 0.01 Ang.
C5A -H5A 1.555 1.555 # 22 Check

PLAT721_ALERT_1_G Bond	Calc	0.97000, Rep	0.96000 Dev...	0.01 Ang.
C5B	-H5F	1.555	1.555	# 27 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd)				1.13 Ratio
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C3	--C5A			1.92 Ang.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.	#			2 Note
C H3				
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed				! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).				2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600			6 Note

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

6 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
9 ALERT type 3 Indicator that the structure quality may be low
13 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

checkCIF publication errors

[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.

[IMAGE] Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

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

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_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 ..... 0.273 Report
RESPONSE: ...
;
_vrf_PLAT417_I
;
PROBLEM: Short Inter D-H..H-D      H4A      ..H4A      1.50 Ang.
RESPONSE: ...
;
_vrf_PLAT973_I
;
```

PROBLEM: Check Calcd Positive Resid. Density on Nil1 2.06 eA-3
 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.

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

Datablock I - ellipsoid plot

