

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 = 0.0272 Å	Wavelength=0.71073	
Cell:	a=20.4341(15)	b=20.4341(15)	c=19.3550(19)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	8081.7(14)	8081.7(14)	
Space group	I 4 2 2	I 4 2 2	
Hall group	I 4 2	I 4 2	
Moiety formula	C56 H80 N32 Ni4 S8 [+ solvent]	C56 H80 N32 Ni4 S8	
Sum formula	C56 H80 N32 Ni4 S8 [+ solvent]	C56 H80 N32 Ni4 S8	
Mr	1692.76	1692.84	
Dx, g cm ⁻³	0.696	0.696	
Z	2	2	
Mu (mm ⁻¹)	0.590	0.590	
F000	1760.0	1760.0	
F000'	1764.96		
h,k,lmax	26,26,25	26,26,25	
Nref	4605[2593]	4581	
Tmin,Tmax	0.809,0.838		
Tmin'	0.745		
Correction method= Not given			
Data completeness=	1.77/0.99	Theta(max)= 27.349	
R(reflections)=	0.1086(2301)	wR2(reflections)= 0.3618(4581)	
S =	1.224	Npar= 103	

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**

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Ni01 2.07 eA-3

[IMAGE] **Alert level B**

SHFSU01_ALERT_2_B The absolute value of parameter shift to su ratio > 0.10

Absolute value of the parameter shift to su ratio given 0.141

Additional refinement cycles may be required.

PLAT080_ALERT_2_B	Maximum Shift/Error	0.14	Why ?
PLAT084_ALERT_3_B	High wR2 Value (i.e. > 0.25)	0.36	Report
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of	C5	Check
PLAT242_ALERT_2_B	Low 'MainMol' Ueq as Compared to Neighbors of	C3	Check
PLAT341_ALERT_3_B	Low Bond Precision on C-C Bonds	0.0272	Ang.
PLAT360_ALERT_2_B	Short C(sp3)-C(sp3) Bond C5 - C6	1.28	Ang.
PLAT360_ALERT_2_B	Short C(sp3)-C(sp3) Bond C5 - C7	1.28	Ang.

[IMAGE] **Alert level C**

STRVA01_ALERT_4_C Flack test results are ambiguous.

From the CIF: _refine_ls_abs_structure_Flack 0.550

From the CIF: _refine_ls_abs_structure_Flack_su 0.060

PLAT082_ALERT_2_C	High R1 Value	0.11	Report
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.26	Report
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.8	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range	4.8	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for S1 --C4	5.3	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for N3 --C4	6.7	s.u.
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.3	Note
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn H1 ..H6C	1.85	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
PLAT761_ALERT_1_C	CIF Contains no X-H Bonds		Please Check
PLAT762_ALERT_1_C	CIF Contains no X-Y-H or H-Y-H Angles		Please Check
PLAT907_ALERT_2_C	Flack x > 0.5, Structure Needs to be Inverted? .	0.55	Check
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	1	Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	1	Check
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Info

[IMAGE] **Alert level G**

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	3	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 .	0.550	Note
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	1	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C5	Check
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure	!	Info
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	33	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	5	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
22 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 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

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_PLAT973_I
;
PROBLEM: Check Calcd Positive Resid. Density on      Ni01      2.07 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

