

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 = 0.0019 Å

Wavelength=0.71073

Cell: a=8.9541(3) b=14.1570(4) c=16.8972(5)
 alpha=104.278(1) beta=98.592(1) gamma=97.958(1)
Temperature: 100 K

	Calculated	Reported
Volume	2017.85(11)	2017.85(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C36 H44 Ni P S, C2 F6 N O4 S2	?
Sum formula	C38 H44 F6 N Ni O4 P S3	C38 H44 F6 N Ni O4 P S3
Mr	878.58	878.60
Dx,g cm-3	1.446	1.446
Z	2	2
Mu (mm-1)	0.743	0.743
F000	912.0	912.0
F000'	914.07	
h,k,lmax	12,19,23	12,19,23
Nref	11869	11759
Tmin,Tmax	0.839,0.911	0.700,0.746
Tmin'	0.740	

Correction method= # Reported T Limits: Tmin=0.700 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.991

Theta(max)= 30.096

R(reflections)= 0.0299(10418)

wR2(reflections)= 0.0824(11759)

S = 1.013

Npar= 650

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 B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).	20	Note
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Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.7	Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C24	Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.3	Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	20	Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers	1	Check

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	2	Note
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)	0.001	Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT300_ALERT_4_G Atom Site Occupancy of S2 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of S20 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F100 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F101 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F102 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F500 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F501 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F502 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of O40 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of O41 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of O200 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of O201 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C37 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C370 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of S10 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of S100 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F200 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F201 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F202 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F400 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F401 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F402 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of O5 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C36 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C360 Constrained at	0.5	Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1)	8%	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	7.50	Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 3	7.50	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact F501 ..C23	2.95	Ang.
	x,y,z =	1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	1	Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group #	30	Check

PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms	! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints	1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	72 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF	1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...	6 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	18 Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 7 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
 39 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

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_PLAT220_I
;
PROBLEM: Non-Solvent  Resd 1  C    Ueq(max)/Ueq(min) Range          3.7 Ratio
RESPONSE: ...
;
_vrf_PLAT242_I
;
PROBLEM: Low      'MainMol' Ueq as Compared to Neighbors of      C24 Check
RESPONSE: ...
;
_vrf_PLAT250_I
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.3 Note
RESPONSE: ...
;
_vrf_PLAT911_I
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      20 Report
RESPONSE: ...
;
_vrf_PLAT934_I
;
PROBLEM: Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....      1 Check
RESPONSE: ...
;
# end Validation Reply Form
```

It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

