

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:	C-C = 0.0023 A	Wavelength=0.71073
Cell:	a=7.3219(3)	b=15.4319(7) c=16.2478(6)
	alpha=111.406(4)	beta=100.879(3) gamma=98.313(4)
Temperature:	100 K	
	Calculated	Reported
Volume	1632.10(13)	1632.10(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C34 H34 N4 Ni O4 S4	C34 H34 N4 Ni O4 S4
Sum formula	C34 H34 N4 Ni O4 S4	C34 H34 N4 Ni O4 S4
Mr	749.58	749.60
Dx,g cm-3	1.525	1.525
Z	2	2
Mu (mm-1)	0.897	0.897
F000	780.0	780.0
F000'	781.91	
h,k,lmax	9,21,22	9,20,21
Nref	8654	7895
Tmin,Tmax	0.806,0.914	0.890,1.000
Tmin'	0.764	

Correction method= # Reported T Limits: Tmin=0.890 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.912	Theta(max)= 28.990
R(reflections)= 0.0281(6813)	wR2(reflections)= 0.0697(7895)
S = 1.015	Npar= 434

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 G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ni --S1 .	6.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ni --S3 .	8.0	s.u.
PLAT794_ALERT_5_G	Tentative Bond Valency for Ni (III) .	2.76	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	2	Note
PLAT883_ALERT_1_G	No Info for _atom_sites_solution_primary		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	745	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	14	Info

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

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

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.

