

# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: ws31lt

---

Bond precision:	C-C = 0.0027 Å	Wavelength=0.71073
Cell:	a=8.3940(17)	b=9.3500(19)      c=13.675(3)
	alpha=82.26(3)	beta=73.44(3)      gamma=82.14(3)
Temperature:	100 K	
	Calculated	Reported
Volume	1013.9(4)	1013.9(4)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C20 H24 Fe N5 O3 S	C20 H24 Fe N5 O3 S
Sum formula	C20 H24 Fe N5 O3 S	C20 H24 Fe N5 O3 S
Mr	470.35	470.35
Dx,g cm-3	1.541	1.541
Z	2	2
Mu (mm-1)	0.874	0.880
F000	490.0	490.0
F000'	491.09	
h,k,lmax	11,13,19	11,13,19
Nref	5965	5929
Tmin,Tmax		0.974,0.991
Tmin'		

Correction method= # Reported T Limits: Tmin=0.974 Tmax=0.991  
AbsCorr = MULTI-SCAN

Data completeness= 0.994      Theta(max)= 30.070

R(reflections)= 0.0401( 5269)      wR2(reflections)= 0.1123( 5929)

S = 1.074      Npar= 277

---

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

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu	
	not performed for this radiation type.	
PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2 Note
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	2 Report
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal .....	0.03000 Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe1 -- S1 ..	8.5 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe1 -- N1 ..	5.3 su
PLAT793_ALERT_4_G	The Model has Chirality at N1 (Centro SPGR)	S Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	1 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note
PLAT984_ALERT_1_G	The Fe-f' = 0.346 Deviates from the B&C-Value	0.348 Check

---

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  
11 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 ALERT type 2 Indicator that the structure model may be wrong or deficient  
1 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
2 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*, 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.

---

