

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: I

Bond precision:	C-C = 0.0098 Å	Wavelength=0.71073
Cell:	a=7.6045(18)	b=11.712(3) c=11.841(3)
	alpha=86.297(8)	beta=86.760(8) gamma=81.079(9)
Temperature:	296 K	
	Calculated	Reported
Volume	1038.5(4)	1038.5(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H19 Cl Fe N2 O S	C24 H19 Cl Fe N2 O S
Sum formula	C24 H19 Cl Fe N2 O S	C24 H19 Cl Fe N2 O S
Mr	474.77	474.77
Dx,g cm-3	1.518	1.518
Z	2	2
Mu (mm-1)	0.974	0.974
F000	488.0	488.0
F000'	489.37	
h,k,lmax	9,14,14	9,14,14
Nref	4087	4044
Tmin,Tmax	0.829,0.873	0.779,0.876
Tmin'	0.769	

Correction method= # Reported T Limits: Tmin=0.779 Tmax=0.876
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 26.000

R(reflections)= 0.0662(1893) wR2(reflections)= 0.1843(4044)

S = 0.995 Npar= 271

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 C

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	47%	Check
PLAT234_ALERT_4_C	Large Hirshfeld Difference C7 --C8 .	0.17	Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Fel Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00975	Ang.
PLAT414_ALERT_2_C	Short Intra D-H..H-X H2A ..H24	1.99	Ang.
	x,y,z =	1_555	Check



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (II) .	2.18	Info
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2018	Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 3 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 2 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
 2 ALERT type 5 Informative message, check
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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.

Datablock I - ellipsoid plot

