

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: ld41a_a

Bond precision: C-C = 0.0032 Å Wavelength=0.71073

Cell: a=14.122(3) b=13.889(3) c=13.470(3)
 alpha=90 beta=118.40(3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2324.0(11)	2324.1(10)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C22 H28 Fe N5 O4 S	?
Sum formula	C22 H28 Fe N5 O4 S	C22 H28 Fe N5 O4 S
Mr	514.40	514.40
Dx,g cm-3	1.470	1.470
Z	4	4
Mu (mm-1)	0.773	0.778
F000	1076.0	1076.0
F000'	1078.24	
h,k,lmax	20,20,19	18,18,18
Nref	7897	6297
Tmin,Tmax	0.982,0.992	0.977,0.992
Tmin'	0.977	

Correction method= # Reported T Limits: Tmin=0.977 Tmax=0.992
AbsCorr = MULTI-SCAN

Data completeness= 0.797 Theta(max)= 31.767

R(reflections)= 0.0408(5792) wR2(reflections)= 0.1118(6297)

S = 1.073 Npar= 301

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

PLAT029_ALERT_3_B	_diffn_measured_fraction_theta_full	value Low	.	0.953	Note
PLAT417_ALERT_2_B	Short Inter D-H..H-D	H1	.. H4B	..	1.87 Ang.

Alert level C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.32	Report
PLAT220_ALERT_2_C	Non-Solvent Resd 1	C Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT222_ALERT_3_C	Non-Solvent Resd 1	H Uiso(max)/Uiso(min) Range	4.3	Ratio
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H7	.. S1	..	2.93 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H20C	.. O2	..	2.62 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H7	.. S1	..	2.93 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H20C	.. O2	..	2.62 Ang.

Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu	not performed for this radiation type.			
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	3	Report	
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range	Identical	?	Check	
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1 -- S1	..	10.5 s.u.	
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1 -- N2	..	5.3 s.u.	
PLAT793_ALERT_4_G	The Model has Chirality at N1	(Centro SPGR)	R	Verify	
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax	Differ	2	Units	
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax	Differ	2	Units	
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
2 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
5 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

