

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_2609

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: exp_2609

Bond precision: C-C = 0.0027 Å Wavelength=1.54184

Cell: a=5.9748 (2) b=7.8641 (4) c=16.8240 (7)
 alpha=89.999 (4) beta=80.991 (3) gamma=68.477 (4)
Temperature: 173 K

	Calculated	Reported
Volume	724.89 (6)	724.89 (6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C14 H17 N O S2	C14 H17 N O S2
Sum formula	C14 H17 N O S2	C14 H17 N O S2
Mr	279.41	279.40
Dx, g cm ⁻³	1.280	1.280
Z	2	2
Mu (mm ⁻¹)	3.224	3.224
F000	296.0	296.0
F000'	297.97	
h, k, lmax	7, 9, 20	7, 9, 20
Nref	2592	2532
Tmin, Tmax	0.454, 0.492	0.520, 1.000
Tmin'	0.310	

Correction method= # Reported T Limits: Tmin=0.520 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.977 Theta(max)= 67.080

R(reflections)= 0.0317 (2384)	wR2(reflections)=
S = 1.062	0.0889 (2532)
Npar= 165	

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

PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE. 293 Degree

 Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.976 Why?
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.597 60 Report

 Alert level G

PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 92% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 48 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.5 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 6 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected
- 1 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
5 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 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_PLAT196_exp_2609
;
PROBLEM: No TEMP record and _measurement_temperature .NE. 293 Degree
RESPONSE: ...
;
_vrf_PLAT029_exp_2609
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low . 0.976 Why?
RESPONSE: ...
;
_vrf_PLAT220_exp_2609
;
PROBLEM: NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
RESPONSE: ...
;
```

_vrf_PLAT911_exp_2609

;

PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.597 60 Report

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.

PLATON version of 06/07/2023; check.def file version of 30/06/2023

