

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) c2c

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: c2c

Bond precision: C-C = 0.0030 Å Wavelength=0.71073

Cell: a=11.4919(4) b=13.3354(5) c=11.8054(6)
 alpha=90 beta=110.904(2) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	1690.09(12)	1690.09(12)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C20 H18 O S2	C20 H18 O S2
Sum formula	C20 H18 O S2	C20 H18 O S2
Mr	338.46	338.46
Dx, g cm ⁻³	1.330	1.330
Z	4	4
Mu (mm ⁻¹)	0.317	0.317
F000	712.0	712.0
F000'	713.23	
h, k, lmax	14, 16, 14	14, 16, 14
Nref	1798	1747
Tmin, Tmax	0.948, 0.996	0.865, 0.970
Tmin'	0.864	

Correction method= # Reported T Limits: Tmin=0.865 Tmax=0.970
AbsCorr = MULTI-SCAN

Data completeness= 0.972 Theta(max)= 26.690

R(reflections)= 0.0469(1377)

wR2(reflections)=
0.1175(1747)

S = 1.038

Npar= 107

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**

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full value Low .	0.972	Why?
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	8.245	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	5	Report

● **Alert level G**

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT300_ALERT_4_G	Atom Site Occupancy of H3A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3B Constrained at	0.5 Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C2 - C3 .	1.53 Ang.
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	45 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	9 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
- 0 **ALERT level B** = A potentially serious problem, consider carefully
- 3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 7 **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
 - 4 ALERT type 3 Indicator that the structure quality may be low
 - 3 ALERT type 4 Improvement, methodology, query or suggestion
 - 1 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.

PLATON version of 19/02/2022; check.def file version of 19/02/2022

