

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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 = 0.0056 A Wavelength=0.71073

Cell: a=13.6934(5) b=19.3166(6) c=7.4283(3)
 alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	1964.86(12)	1964.86(12)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C24 H20 O2 S2	?
Sum formula	C24 H20 O2 S2	C24 H20 O2 S2
Mr	404.52	404.52
Dx,g cm-3	1.367	1.367
Z	4	4
Mu (mm-1)	0.289	0.289
F000	848.0	848.0
F000'	849.31	
h,k,lmax	17,25,9	17,25,9
Nref	2267	2262
Tmin,Tmax	0.878,0.901	0.820,0.840
Tmin'	0.876	

Correction method= # Reported T Limits: Tmin=0.820 Tmax=0.840
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 27.500

R(reflections)= 0.0828(2012) wR2(reflections)= 0.2685(2262)

S = 1.092 Npar= 128

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

DIFMX01_ALERT_2_B The maximum difference density is > 0.1*ZMAX*1.00
 _refine_diff_density_max given = 2.412
 Test value = 1.600
PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 2.41 eA-3
PLAT230_ALERT_2_B Hirshfeld Test Diff for C12 -- C13 .. 8.3 su

🟡 Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
 The relevant atom site should be identified.
RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
 Weighted R factor given 0.269
PLAT048_ALERT_1_C MoietyFormula Not Given Please Do !
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.27 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ... 3.85 Report
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.0056 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H13C .. H13C .. 2.12 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 3.610 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 3 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much smaller I(calc) . 7 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 23.08
PLAT971_ALERT_2_C Check Calcd Residual Density 2.30A From C13 2.49 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.21A From C13 2.37 eA-3

🟡 Alert level G

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.16 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 8.02 Why ?
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ... 2 Report

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
14 **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
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 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
-

checkCIF publication errors

🔴 Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
 _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
 _publ_contact_author_phone are all missing.
 At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
 e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).

PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

7 **ALERT level A** = Data missing that is essential or data in wrong format

1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

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_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
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;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form

```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 21/04/2015; check.def file version of 09/03/2015

Datablock I - ellipsoid plot

