

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 = 0.0103 Å Wavelength=1.54178

Cell: a=5.0613(4) b=13.3347(10) c=22.6731(18)
 alpha=90 beta=90 gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	1530.2(2)	1530.2(2)
Space group	P 2 21 21	P 2 21 21
Hall group	P 2bc 2	P 2bc 2
Moiety formula	C16 H16 N2 O2 S	C16 H16 N2 O2 S
Sum formula	C16 H16 N2 O2 S	C16 H16 N2 O2 S
Mr	300.37	300.37
Dx,g cm-3	1.304	1.304
Z	4	4
Mu (mm-1)	1.927	1.927
F000	632.0	632.0
F000'	635.04	
h,k,lmax	5,14,25	5,14,25
Nref	2207[1328]	2206
Tmin,Tmax	0.891,0.981	0.485,0.753
Tmin'	0.667	

Correction method= MULTI-SCAN

Data completeness= 1.66/1.00 Theta(max)= 58.901

R(reflections)= 0.0515(1792) wR2(reflections)= 0.1273(2206)

S = 1.044 Npar= 194

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

Crystal system given = orthorhombic
THETM01_ALERT_3_B The value of $\sin(\theta_{\max})/\lambda$ is less than 0.575
Calculated $\sin(\theta_{\max})/\lambda = 0.5554$
PLAT023_ALERT_3_B Resolution (too) Low [$\sin(\theta)/\lambda < 0.6$].. 58.90 Degree
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.0103 Ang.

Alert level C

PLAT089_ALERT_3_C Poor Data / Parameter Ratio ($Z_{\max} < 18$) 6.85 Note
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for C3 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for S1 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C10 Check
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist. C10 -C15 1.36 Ang.
PLAT334_ALERT_2_C Small Average Benzene C-C Dist. C4 -C8 1.37 Ang.

Alert level G

PLAT033_ALERT_4_G Flack x Value Deviates $> 2\sigma$ from Zero 0.140
PLAT128_ALERT_4_G Alternate Setting for Input Space Group P2121 P2121 Note
PLAT791_ALERT_4_G The Model has Chirality at C1 S Verify
PLAT791_ALERT_4_G The Model has Chirality at C2 R Verify

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected
- 0 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
4 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
-

checkCIF publication errors

Alert level A

PUBL002_ALERT_1_A The contact author's address is missing,
_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.

- 7 **ALERT level A** = Data missing that is essential or data in wrong format
0 **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.

```
# start Validation Reply Form
_vrf_PUBL002_GLOBAL
;
PROBLEM: The contact author's address is 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: ...
;
_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 24/07/2014; check.def file version of 24/07/2014

Datablock I - ellipsoid plot

