

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 = 0.0026 Å Wavelength=0.71073

Cell: a=7.1500(3) b=25.5032(9) c=22.9477(8)
 alpha=90 beta=93.571(1) gamma=90

Temperature: 90 K

	Calculated	Reported
Volume	4176.3(3)	4176.3(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 H18 O6 S2	1(C24 H18 O6 S2)
Sum formula	C24 H18 O6 S2	C24 H18 O6 S2
Mr	466.50	466.50
Dx,g cm-3	1.484	1.484
Z	8	8
Mu (mm-1)	0.296	0.296
F000	1936.0	1936.0
F000'	1938.94	
h,k,lmax	10,36,32	10,36,32
Nref	12798	12747
Tmin,Tmax	0.982,0.988	0.691,0.746
Tmin'	0.943	

Correction method= # Reported T Limits: Tmin=0.691 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 30.554

R(reflections)= 0.0506(9186) wR2(reflections)= 0.1272(12747)

S = 1.047 Npar= 663

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.14	Report
PLAT213_ALERT_2_C	Atom O2 has ADP max/min Ratio	3.1	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 2 C Ueq(max) / Ueq(min) Range	3.1	Ratio
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.2	Note
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.445	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	8	Report



Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	13%	Note
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 2)	13%	Note
PLAT793_ALERT_4_G	Model has Chirality at C15A (Centro SPGR)		R Verify
PLAT793_ALERT_4_G	Model has Chirality at C22A (Centro SPGR)		R Verify
PLAT793_ALERT_4_G	Model has Chirality at C39A (Centro SPGR)		S Verify
PLAT793_ALERT_4_G	Model has Chirality at C46A (Centro SPGR)		S Verify
PLAT793_ALERT_4_G	Model has Chirality at C15B (Centro SPGR)		S Verify
PLAT793_ALERT_4_G	Model has Chirality at C22B (Centro SPGR)		S Verify
PLAT793_ALERT_4_G	Model has Chirality at C39B (Centro SPGR)		R Verify
PLAT793_ALERT_4_G	Model has Chirality at C46B (Centro SPGR)		R Verify
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	43	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.2	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	19	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	1	Check

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

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.

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: ...
;
_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 you wish to submit your CIF for publication in IUCrData 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 22/04/2020; check.def file version of 09/03/2020

Datablock I - ellipsoid plot

