

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 = 0.0158 Å Wavelength=0.71073

Cell: a=18.380(4) b=10.170(2) c=6.0800(12)
 alpha=90 beta=90 gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	1136.5(4)	1136.5(4)
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C12 H17 N O2	?
Sum formula	C12 H17 N O2	C12 H17 N O2
Mr	207.27	207.26
Dx,g cm-3	1.211	1.211
Z	4	4
Mu (mm-1)	0.082	0.082
F000	448.0	448.0
F000'	448.20	
h,k,lmax	20,11,6	20,11,6
Nref	1639[911]	1348
Tmin,Tmax	0.984,0.984	0.991,0.992
Tmin'	0.984	

Correction method= # Reported T Limits: Tmin=0.991 Tmax=0.992
AbsCorr = MULTI-SCAN

Data completeness= 1.48/0.82 Theta(max)= 23.248

R(reflections)= 0.0851(884) wR2(reflections)= 0.1861(1348)

S = 1.166 Npar= 138

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

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 [$\sin(\theta)/\lambda < 0.6$].. 23.25 Degree
PLAT029_ALERT_3_B $\text{_diffraction_measured_fraction_theta_full}$ value Low . 0.952 Why?
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01582 Ang.

Alert level C

ABSTY02_ALERT_1_C An $\text{_exptl_absorpt_correction_type}$ has been given without
a literature citation. This should be contained in the
 $\text{_exptl_absorpt_process_details}$ field.
Absorption correction given as multi-scan
STRVA01_ALERT_4_C Flack parameter is too small
From the CIF: $\text{_refine_ls_abs_structure_Flack}$ -1.700
From the CIF: $\text{_refine_ls_abs_structure_Flack_su}$ 1.000
PLAT048_ALERT_1_C MoietyFormula Not Given (or Incomplete) Please Check
PLAT089_ALERT_3_C Poor Data / Parameter Ratio ($Z_{\max} < 18$) 6.28 Note
PLAT911_ALERT_3_C Missing FCF Refl Between θ_{\min} & $\theta_{\max}/L = 0.555$ 44 Report
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage 66 %
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 12 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 1.000 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 3 Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp²)-Methyl Moiety C4 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints 91 Note
PLAT883_ALERT_1_G No Info/Value for $\text{_atom_sites_solution_primary}$. Please Do !
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 1.47 Check

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
4 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected
- 3 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
8 ALERT type 3 Indicator that the structure quality may be low
6 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,
 $\text{_publ_contact_author_name}$ and $\text{_publ_contact_author_address}$.
PUBL005_ALERT_1_A $\text{_publ_contact_author_email}$, $\text{_publ_contact_author_fax}$ and
 $\text{_publ_contact_author_phone}$ are all missing.
At least one of these should be present.
PUBL006_ALERT_1_A $\text{_publ_requested_journal}$ 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
```

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;
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 07/08/2019; check.def file version of 30/07/2019

