

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_8594

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: exp_8594

Bond precision:	C-C = 0.0035 A	Wavelength=1.54184
Cell:	a=25.9663(6)	b=10.0851(2) c=27.9727(7)
	alpha=90	beta=101.769(3) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	7171.3(3)	7171.3(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C76 H76 [+ solvent]	2(C76 H76)
Sum formula	C76 H76 [+ solvent]	C152 H152
Mr	989.37	1978.73
Dx,g cm-3	0.916	0.916
Z	4	2
Mu (mm-1)	0.384	0.384
F000	2128.0	2128.0
F000'	2133.25	
h,k,lmax	30,11,33	30,11,33
Nref	12379	12048
Tmin,Tmax	0.912,0.985	0.661,1.000
Tmin'	0.891	
Correction method= # Reported T Limits: Tmin=0.661 Tmax=1.000		
AbsCorr = MULTI-SCAN		
Data completeness=	0.973	Theta(max)= 65.712
R(reflections)=	0.0665(8791)	wR2(reflections)= 0.1756(12048)
S =	0.958	Npar= 733

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

PLAT410_ALERT_2_B Short Intra H...H Contact H00B ..H017 . 1.81 Ang.
x,y,z = 1_555 Check

Alert level C

PLAT018_ALERT_1_C _diffn_measured_fraction_theta_max .NE. *_full ! Check
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range 3.5 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C013 --C01W . 6.5 s.u.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C01Q Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 5.703 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.150 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.591 331 Report

Alert level G

PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2.00 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C022 Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C023 Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C024 Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1 Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2 Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3 Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02G Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02H Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02I Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02J Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02K Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02L Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02M Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02N Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02O Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1A Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1B Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1C Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2A Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2B Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2C Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3A Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3B Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3C Constrained at 0.3 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 4% Note
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C004 -C007 . 1.42 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 151 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 55% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 37 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
37 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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7 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
27 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
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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.
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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
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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

