

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 = 0.0145 A	Wavelength=0.71073
Cell:	a=25.9703(19)	b=9.1157(7) c=11.3951(8)
	alpha=90	beta=90 gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	2697.7(3)	2697.6(3)
Space group	P m n 21	P m n 21
Hall group	P 2ac -2	P 2ac -2
Moiety formula	C43 H27 Co3 O16	0.5(C86 H54 Co6 O32)
Sum formula	C43 H27 Co3 O16	C43 H27 Co3 O16
Mr	976.44	976.43
Dx,g cm-3	1.202	1.202
Z	2	2
Mu (mm-1)	0.968	0.968
F000	988.0	988.0
F000'	990.58	
h,k,lmax	31,11,13	31,11,13
Nref	5128[2703]	5113
Tmin,Tmax	0.770,0.800	0.773,0.808
Tmin'	0.755	
Correction method=	# Reported T Limits: Tmin=0.773 Tmax=0.808	
AbsCorr =	MULTI-SCAN	
Data completeness=	1.89/1.00	Theta(max)= 25.495
R(reflections)=	0.0674(4716)	wR2(reflections)= 0.1780(5113)
S =	1.090	Npar= 293

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 A

PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

Alert level B

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Col Check
PLAT430_ALERT_2_B Short Inter D...A Contact 04 ..04 . 2.77 Ang.
1-x,y,z = 3_655 Check

Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.490
From the CIF: _refine_ls_abs_structure_Flack_su 0.050
PLAT213_ALERT_2_C Atom O8 has ADP max/min Ratio 3.5 oblate
PLAT220_ALERT_2_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 4.7 Ratio
PLAT222_ALERT_3_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 5.5 Ratio
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.01452 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C1 - C2 . 1.53 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C5 - C8 . 1.54 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C43 H27 Co3 O16
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers 1 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.65A From OlW 0.72 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.01A From O4 0.56 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.46A From OlW -0.59 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H22 -0.39 eA-3
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
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 3 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 11.45 Why ?
PLAT115_ALERT_5_G ADDSYM Detects Noncrystallographic Inversion ... 91% Check
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
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2WA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2WB Constrained at 0.5 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 2 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.10 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Col (II) . 2.16 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 95 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check

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

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

14 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
9 ALERT type 4 Improvement, methodology, query or suggestion
5 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,
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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: ...
;
_vrf_PLAT602_I
;
PROBLEM: VERY LARGE Solvent Accessible VOID(S) in Structure      ! Info
RESPONSE: ...
;
# end Validation Reply Form

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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 13/12/2018; check.def file version of 11/12/2018

