

# 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

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Bond precision:	C-C = 0.0088 A	Wavelength=0.71073
Cell:	a=11.2077(13)	b=18.930(2)      c=13.1237(15)
	alpha=90	beta=98.426(2)      gamma=90
Temperature:	298 K	
	Calculated	Reported
Volume	2754.3(5)	2754.4(5)
Space group	P 21/n	P21/n
Hall group	-P 2yn	?
Moiety formula	C26 H20 Co N6 O4, C2 O2, H2 O	?
Sum formula	C28 H22 Co N6 O7	C28 H22 Co N6 O7
Mr	613.45	613.45
Dx,g cm-3	1.479	1.479
Z	4	4
Mu (mm-1)	0.681	0.681
F000	1260.0	1260.0
F000'	1261.93	
h,k,lmax	13,22,15	13,22,15
Nref	5124	5124
Tmin,Tmax	0.885,0.891	0.887,0.893
Tmin'	0.885	
Correction method=	# Reported T Limits: Tmin=0.887 Tmax=0.893	
AbsCorr =	MULTI-SCAN	
Data completeness=	1.000	Theta(max)= 25.500
R(reflections)=	0.0691( 4299)	wR2(reflections)= 0.2367( 5124)
S =	1.127	Npar= 381

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**test-name\_ALERT\_alert-type\_alert-level.**  
Click on the hyperlinks for more details of the test.

PLAT420\_ALERT 2 B D-H Without Acceptor 06 --H6A . Please Check

PLAT048_ALERT_1_C	MoietyFormula Not Given (or Incomplete) .....			Please Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....		3.40	Report
PLAT125_ALERT_4_C	No '_symmetry_space_group_name_Hall' Given .....			Please Do !
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	05	0.154	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	07	0.149	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	06	0.265	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....		0.00879	Anq.

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	5	Report
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please	Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	4	Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.14	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	6.17	Why ?
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed	Check
PLAT344_ALERT_2_G	Unusual Angle Range in Solvent/Ion for	C27	Check
PLAT344_ALERT_2_G	Unusual sp? Angle Range in Solvent/Ion for	C28	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O5	92.3	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O7	89.6	Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact O5 ..C6	3.01	Ang.
	x,y,z =	1_555	Check
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C28 --C28	2.02	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	118	Check
	O7 -C28 -C28 1.555 1.555 3.667	44.00	Deg.
PLAT794_ALERT_5_G	Tentative Bond Valency for Col (III) .	3.69	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	32	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2018	Note

```
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
18 ALERT level G = General information/check it is not something unexpected
```

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3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

```

## checkCIF publication errors

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.



#### Alert level G

PUBL017\_ALERT\_1\_G The `_publ_section_references` section is missing or empty.

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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

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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.

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**PLATON version of 17/03/2019; check.def file version of 04/03/2019**

