

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 8

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: 8

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Bond precision:	C-C = 0.0020 Å	Wavelength=0.71073
Cell:	a=6.4439 (4)	b=5.8690 (3)      c=26.8276 (19)
	alpha=90	beta=95.696 (6)      gamma=90
Temperature:	93 K	
	Calculated	Reported
Volume	1009.59 (11)	1009.59 (11)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C8 H3 Cl4 N O2	C8 H3 Cl4 N O2
Sum formula	C8 H3 Cl4 N O2	C8 H3 Cl4 N O2
Mr	286.91	286.93
Dx, g cm <sup>-3</sup>	1.888	1.888
Z	4	4
Mu (mm <sup>-1</sup> )	1.145	1.143
F000	568.0	568.0
F000'	570.55	
h, k, lmax	8, 7, 35	8, 7, 32
Nref	2479	2148
Tmin, Tmax	0.892, 0.977	0.802, 0.977
Tmin'	0.892	

Correction method= # Reported T Limits: Tmin=0.802 Tmax=0.977  
AbsCorr = MULTI-SCAN

Data completeness= 0.866      Theta(max)= 28.139

R(reflections)= 0.0303 ( 1972)	wR2(reflections)= 0.0862 ( 2148)
S = 1.006	Npar= 140

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

## PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 2.07 Report

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2	Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT431_ALERT_2_G	Short Inter HL..A Contact C14 ..09 .	2.94	Ang.
	1+x,-1+y,z =	1_645	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C2 .	2.92	Ang.
	1-x,-1/2+y,1/2-z =	2_645	Check
PLAT793_ALERT_4_G	Model has Chirality at C3 (Centro SPGR)		R Verify
PLAT793_ALERT_4_G	Model has Chirality at C8 (Centro SPGR)		S Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	1	Note
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	303	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	4.6	Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	3	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.	3	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	9	Info

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0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
14 ALERT level G = General information/check it is not something unexpected
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- ```
1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

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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.

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**PLATON version of 28/11/2022; check.def file version of 09/08/2022**

