

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

Bond precision:	C-C = 0.0105 Å	Wavelength=0.71073	
Cell:	a=12.3186(15)	b=22.916(2)	c=7.9518(13)
	alpha=90	beta=108.8300	gamma=90
Temperature:	298 K		
	Calculated	Reported	
Volume	2124.6(5)	2124.6(5)	
Space group	P 21/c	P21/c	
Hall group	-P 2ybc	?	
Moiety formula	C20 H16 Br2 Cl2 Co N2 O2	?	
Sum formula	C20 H16 Br2 Cl2 Co N2 O2	C20 H16 Br2 Cl2 Co N2 O2	
Mr	605.98	606.00	
Dx, g cm ⁻³	1.895	1.895	
Z	4	4	
Mu (mm ⁻¹)	4.840	4.841	
F000	1188.0	1188.0	
F000'	1188.72		
h, k, lmax	14, 27, 9	14, 27, 9	
Nref	3794	2979	
Tmin, Tmax	0.395, 0.439	0.444, 0.493	
Tmin'	0.365		

Correction method= # Reported T Limits: Tmin=0.444 Tmax=0.493
AbsCorr = MULTI-SCAN

Data completeness= 0.785 Theta(max)= 25.130

R(reflections)= 0.0434(1478) wR2(reflections)= 0.0813(2979)

S = 0.771 Npar= 262

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

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	N2	--	C18	..	13.4 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C18	--	C19	..	8.3 s.u.
PLAT360_ALERT_2_B	Short C(sp3)-C(sp3) Bond	C18	-	C19	..	1.30 Ang.

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <= 2.00
Goodness of fit given = 0.771

PLAT018_ALERT_1_C	_diffrn_measured_fraction_theta_max .NE. *_full				! Check
PLAT048_ALERT_1_C	MoietyFormula Not Given (or Incomplete)				Please Check
PLAT125_ALERT_4_C	No '_symmetry_space_group_name_Hall' Given				Please Do !
PLAT213_ALERT_2_C	Atom C18			has ADP max/min Ratio	3.3 prolat
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C			Ueq(max)/Ueq(min) Range	4.3 Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	N2	--	C17	.. 5.5 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C18	--	C20	.. 0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C19	--	C20	.. 0.25 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of			C18	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of			C19	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of			N2	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds				0.0105 Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond	C18	-	C20	.. 1.36 Ang.

Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF				Please Do !
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as				mixed Check
PLAT145_ALERT_4_G	s.u. on beta Small or Missing				0.0000 Degree
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL				2014 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
5 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,
_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.

 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
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
```

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_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 11/08/2016; check.def file version of 04/08/2016

Datablock I - ellipsoid plot

