

# checkCIF (full publication check) running

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Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait ..

# checkCIF/PLATON (full publication check)

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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.

Please wait while processing ....

[report](#)

[Structure factor report](#)

[CIF dictionary](#)

[Interpreting this](#)

## Datablock: 21031ocu

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Bond precision: C-C = 0.0036 A Wavelength=1.54184

Cell: a=12.3348 (7) b=12.8057 (8) c=13.5088 (6)  
alpha=61.803 (6) beta=65.982 (5) gamma=63.355 (6)

Temperature: 150 K

	Calculated	Reported
Volume	1628.48 (19)	1628.5 (2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C38 H30 Br N3 O4	C38 H30 Br N3 O4
Sum formula	C38 H30 Br N3 O4	C38 H30 Br N3 O4
Mr	672.55	672.56
Dx, g cm <sup>-3</sup>	1.372	1.372
Z	2	2
Mu (mm <sup>-1</sup> )	2.084	2.084
F000	692.0	692.0
F000'	692.50	
h, k, lmax	14, 14, 15	14, 14, 15
Nref	5228	5172
Tmin, Tmax	0.740, 0.882	0.615, 0.885
Tmin'	0.489	

Correction method= # Reported T Limits: Tmin=0.615

Tmax=0.885 AbsCorr = ANALYTICAL

Data completeness= 0.989 Theta(max)= 62.717

R(reflections)= 0.0355 ( 4649) wR2(reflections)= 0.0959 ( 5172)

S = 1.034 Npar= 415

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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.

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**Alert level C**

[THETM01 ALERT 3 C](#) The value of  $\sin(\theta_{\max})/\lambda$  is less than 0.590

Calculated  $\sin(\theta_{\max})/\lambda = 0.5764$

[PLAT023 ALERT 3 C](#) Resolution (too) Low [ $\sin(\theta)/\lambda < 0.6$ ].. 0.58 Ang-1

[PLAT220 ALERT 2 C](#) NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.2 Ratio

[PLAT222 ALERT 3 C](#) NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.2 Ratio

[PLAT241 ALERT 2 C](#) High 'MainMol' Ueq as Compared to Neighbors of C15 Check

[PLAT414 ALERT 2 C](#) Short Intra D-H..H-X H2A ..H56 1.96 Ang.

x,y,z = 1\_555

Check

[PLAT420 ALERT 2 C](#) D-H Without Acceptor N2 --H2A . Please Check

[PLAT906 ALERT 3 C](#) Large K Value in the Analysis of Variance ..... 3.472 Check

[PLAT911 ALERT 3 C](#) Missing FCF Refl Between Thmin & STh/L= 0.576 56 Report

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**Alert level G**

[PLAT007 ALERT 5 G](#) Number of Unrefined Donor-H Atoms ..... 3 Report

[PLAT793 ALERT 4 G](#) Model has Chirality at C2 (Centro SPGR) S Verify

**And 2 other PLAT793 Alerts**

Less ...

[PLAT793 ALERT 4 G](#) Model has Chirality at C3 (Centro SPGR) R Verify

[PLAT793 ALERT 4 G](#) Model has Chirality at C4 (Centro SPGR) S Verify

[PLAT802 ALERT 4 G](#) CIF Input Record(s) with more than 80 Characters 1 Info

[PLAT883 ALERT 1 G](#) No Info/Value for \_atom\_sites\_solution\_primary . Please Do !

[PLAT909 ALERT 3 G](#) Percentage of I>2sig(I) Data at Theta(Max) Still 100% Note

[PLAT933 ALERT 2 G](#) Number of OMIT Records in Embedded .res File ... 5 Note

[PLAT941 ALERT 3 G](#) Average HKL Measurement Multiplicity ..... 2.4 Low

[PLAT965 ALERT 2 G](#) The SHELXL WEIGHT Optimisation has not Converged Please Check

[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

9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

11 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
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  
4 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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## checkCIF publication errors

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### 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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### 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.

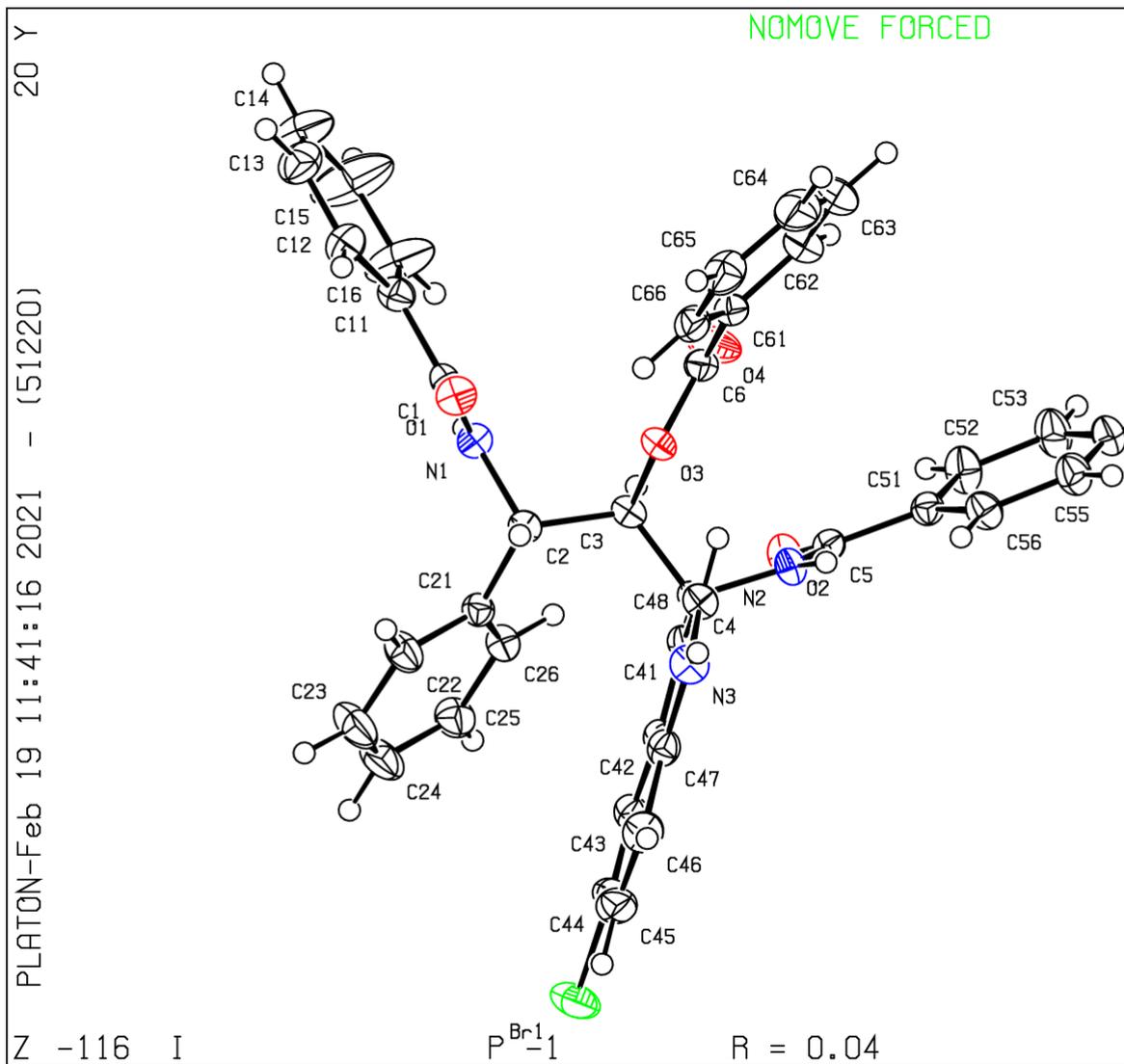
```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
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 05/12/2020; check.def file version of 05/12/2020**

## **Datablock I - ellipsoid plot**



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[Test a new CIF entry](#)