

# 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 = 0.0068 A	Wavelength=0.71073	
Cell:	a=8.8555(16)	b=16.944(3)	c=21.303(3)
	alpha=90	beta=90	gamma=90
Temperature:	294 K		
	Calculated	Reported	
Volume	3196.5(9)	3196.5(9)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C30 H16 Cl2 Cu2 F6 N4 O8	C30 H16 Cl2 Cu2 F6 N4 O8	
Sum formula	C30 H16 Cl2 Cu2 F6 N4 O8	C30 H16 Cl2 Cu2 F6 N4 O8	
Mr	872.47	872.45	
Dx,g cm-3	1.813	1.813	
Z	4	4	
Mu (mm-1)	1.592	1.592	
F000	1736.0	1736.0	
F000'	1740.70		
h,k,lmax	10,20,25	10,20,25	
Nref	5797[ 3280]	5796	
Tmin,Tmax	0.810,0.909	0.780,0.908	
Tmin'	0.775		

Correction method= MULTI-SCAN

Data completeness= 1.77/1.00      Theta(max)= 25.250

R(reflections)= 0.0455( 4701)      wR2(reflections)= 0.1113( 5796)

S = 1.041      Npar= 506

---

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

PLAT094_ALERT_2_B	Ratio of Maximum / Minimum Residual Density ....	6.01	Report
PLAT230_ALERT_2_B	Hirshfeld Test Diff for O2 -- C1 ..	7.7	su
PLAT230_ALERT_2_B	Hirshfeld Test Diff for O6 -- C16 ..	8.7	su

## Alert level C

DIFMX01\_ALERT\_2\_C The maximum difference density is > 0.1\*ZMAX\*0.75  
\_refine\_diff\_density\_max given = 2.318  
Test value = 2.175

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75  
The relevant atom site should be identified.

STRVA01\_ALERT\_4\_C Flack test results are ambiguous.  
From the CIF: \_refine\_ls\_abs\_structure\_Flack 0.614  
From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su 0.017

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18) .....	6.48	Note
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	2.32	eA-3
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for .....	01	Check
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for .....	02	Check
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for .....	05	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for .....	C14	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for .....	C29	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.0068	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact H6 .. H8 ..	1.96	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact H21 .. H23 ..	1.98	Ang.
PLAT922_ALERT_1_C	wR2 in the CIF and FCF Differ by .....	-0.0028	Check
PLAT923_ALERT_1_C	S values in the CIF and FCF Differ by .....	-0.026	Check
PLAT971_ALERT_2_C	Check Calcd Residual Density 1.41A From O6	1.99	eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density 1.38A From O2	1.57	eA-3

## Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	8	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Dimension .....	1	Info
PLAT033_ALERT_4_G	Flack x Value Deviates > 2*sigma from Zero .....	0.614	
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	4	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1 -- O6_a ..	5.5	su
PLAT242_ALERT_2_G	Low Ueq as Compared to Neighbors for .....	C15	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	Percentage =	8 Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	131	Check
	C30B -C29 -C30A 1.555 1.555 1.555	4.30	Deg.
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II) .....	2.29	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu2 (II) .....	2.31	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	90	Note
PLAT909_ALERT_3_G	Percentage of Observed Data at Theta(Max) still	60	%
PLAT910_ALERT_3_G	Missing # of FCF Reflections Below Th(Min) .....	1	Report
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	1	Check

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

3 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
18 **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  
5 **ALERT type 4** Improvement, methodology, query or suggestion  
3 **ALERT type 5** Informative message, check

---

## checkCIF publication errors

---

### Alert level A

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.

---

6 **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_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 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 20/08/2014; check.def file version of 18/08/2014**

