

# 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

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Bond precision:	C-C = 0.0045 A	Wavelength=0.71073	
Cell:	a=9.7197(8)	b=26.883(3)	c=10.0214(9)
	alpha=90	beta=101.848(9)	gamma=90
Temperature:	250 K		
	Calculated	Reported	
Volume	2562.8(4)	2562.7(4)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C26 H32 O6 Ti	C26 H32 O6 Ti	
Sum formula	C26 H32 O6 Ti	C26 H32 O6 Ti	
Mr	488.39	488.42	
Dx,g cm-3	1.266	1.266	
Z	4	4	
Mu (mm-1)	0.371	0.371	
F000	1032.0	1032.0	
F000'	1033.59		
h,k,lmax	12,35,13	12,35,13	
Nref	6365	6352	
Tmin,Tmax	0.961,0.974	0.964,0.979	
Tmin'	0.949		

Correction method= ANALYTICAL

Data completeness= 0.998      Theta(max)= 28.280

R(reflections)= 0.0697( 3566)      wR2(reflections)= 0.1735( 6352)

S = 1.023      Npar= 328

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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

PLAT220_ALERT_2_C	Large Non-Solvent C	Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O4 -- C15 ..	5.5	su
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O5 -- C23B ..	0.16	Ang.
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for .....	C19	Check
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance .....		21.286	Check
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance .....		3.597	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflections Below Th(Min) .....		8	Report

## ● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		10	Note
PLAT005_ALERT_5_G	No <code>_iucr_refine_instructions_details</code> in the CIF		Please Do !	
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Til	-- O6 ..	5.8	su
PLAT301_ALERT_3_G	Main Residue Disorder .....	Percentage =	12	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #		36	Check
	C23A -O5 -C23B	1.555 1.555 1.555	34.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #		42	Check
	C25A -O6 -C25C	1.555 1.555 1.555	38.90	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #		44	Check
	C25B -O6 -C25A	1.555 1.555 1.555	38.30	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #		45	Check
	C25B -O6 -C25C	1.555 1.555 1.555	36.00	Deg.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		8	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	5	Note

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

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

## checkCIF publication errors

### ● Alert level A

PUBL002\_ALERT\_1\_A The contact author's address is missing,  
`_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.

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_PUBL002_GLOBAL
;
PROBLEM: The contact author's address is 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 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 20/08/2014; check.def file version of 18/08/2014**

Datablock I - ellipsoid plot

