

## checkCIF (full publication check) running

## checkCIF/PLATON (full publication check)

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 ....

[CIF dictionary](#)  
[Interpreting this report](#)

[Structure factor report](#)

## Datablock: I

Bond precision: C-C = 0.0040 Å Wavelength=0.71073  
Cell: a=8.1472(6) b=9.9846(7) c=9.3679(6)  
alpha=90 beta=113.994(4) gamma=90  
Temperature: 150 K

	Calculated	Reported
Volume	696.20(9)	696.20(9)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C3 H4 Mn N4 O3, H2 O	C3 H4 Mn N4 O3, H2 O
Sum formula	C3 H6 Mn N4 O4	C3 H6 Mn N4 O4
Mr	217.06	217.06
Dx,g cm-3	2.071	2.071
Z	4	4
Mu (mm-1)	1.877	1.877
F000	436.0	436.0
F000'	437.53	
h,k,lmax	10,12,11	10,12,11
Nref	1417	1418
Tmin,Tmax	0.813,0.928	0.806,0.912
Tmin'	0.813	

Correction method= # Reported T Limits: Tmin=0.806 Tmax=0.912  
AbsCorr = MULTI-SCAN  
Data completeness= 1.001 Theta(max)= 26.367  
R(reflections)= 0.0388( 1162) wR2(reflections)= 0.0935( 1418)  
S = 0.993 Npar= 127

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 C

[RINTA01\\_ALERT\\_3\\_C](#) The value of Rint is greater than 0.12  
Rint given 0.150

### ● Alert level G

<a href="#">PLAT002_ALERT_2_G</a> Number of Distance or Angle Restraints on AtSite	8 Note
<a href="#">PLAT004_ALERT_5_G</a> Polymeric Structure Found with Maximum Dimension	2 Info
<a href="#">PLAT172_ALERT_4_G</a> The CIF-Embedded .res File Contains DFIX Records	7 Report
<a href="#">PLAT720_ALERT_4_G</a> Number of Unusual/Non-Standard Labels .....	4 Note
<a href="#">PLAT764_ALERT_4_G</a> Overcomplete CIF Bond List Detected (Rep/Expd) .	1.20 Ratio
<a href="#">PLAT790_ALERT_4_G</a> Centre of Gravity not Within Unit Cell: Resd. # H2 O	2 Note
<a href="#">PLAT860_ALERT_3_G</a> Number of Least-Squares Restraints .....	8 Note

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 ALERT type 2 Indicator that the structure model may be wrong or deficient  
2 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

---

### ●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.

---

### ●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: ...
```

```

;
_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 21/06/2015; check.def file version of 21/06/2015

## Datablock I - ellipsoid plot

