

# 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

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|                 |                          |                                |
|-----------------|--------------------------|--------------------------------|
| Bond precision: | C-C = 0.0046 A           | Wavelength=0.71073             |
| Cell:           | a=16.0635(7)             | b=13.5669(9)      c=17.4719(7) |
|                 | alpha=90                 | beta=91.639(4)      gamma=90   |
| Temperature:    | 123 K                    |                                |
|                 | Calculated               | Reported                       |
| Volume          | 3806.1(3)                | 3806.1(3)                      |
| Space group     | P 21/c                   | P 1 21/c 1                     |
| Hall group      | -P 2ybc                  | -P 2ybc                        |
| Moiety formula  | C84 H70 Mo2 O4, 2(C7 H8) | C84 H70 Mo2 O4, 2(C7 H8)       |
| Sum formula     | C98 H86 Mo2 O4           | C98 H86 Mo2 O4                 |
| Mr              | 1519.55                  | 1519.54                        |
| Dx,g cm-3       | 1.326                    | 1.326                          |
| Z               | 2                        | 2                              |
| Mu (mm-1)       | 0.384                    | 0.384                          |
| F000            | 1580.0                   | 1580.0                         |
| F000'           | 1573.66                  |                                |
| h,k,lmax        | 24,20,26                 | 24,20,26                       |
| Nref            | 14316                    | 13094                          |
| Tmin,Tmax       | 0.831,0.880              | 0.862,0.902                    |
| Tmin'           | 0.831                    |                                |

Correction method= # Reported T Limits: Tmin=0.862 Tmax=0.902  
AbsCorr = GAUSSIAN

Data completeness= 0.915      Theta(max)= 32.961

R(reflections)= 0.0581( 8969)      wR2(reflections)= 0.1770( 13094)

S = 1.083      Npar= 457

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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.



## Alert level C

PLAT241\_ALERT\_2\_C High

Ueq as Compared to Neighbors for .....

C32 Check



## Alert level G

|   |       |        |
|---|-------|--------|
| PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. | 0.10  | Report |
| PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mol -- C1 ..          | 5.1   | su     |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C43A is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C44A is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C45A is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C46A is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C47A is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C48A is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C49A is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H43A is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H43B is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H43C is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H45A is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H46A is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H47A is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H48A is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H49A is Constrained at  | 0.320 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C43B is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C44B is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C45B is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C46B is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C47B is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C48B is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C49B is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H43D is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H43E is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H43F is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H45B is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H46B is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H47B is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H48B is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H49B is Constrained at  | 0.280 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C43D is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C44C is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C45C is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C46C is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C47C is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C48C is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <C49C is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H43G is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H43H is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H43I is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H44C is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H45C is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H46C is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H47C is Constrained at  | 0.400 | Check  |
| PLAT300_ALERT_4_G Atom Site Occupancy of <H48C is Constrained at  | 0.400 | Check  |
| PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =       | 100   | Note   |
| PLAT304_ALERT_4_G Non-Integer Number of Atoms ( 4.80) in Resd. #  | 2     | Check  |
| PLAT304_ALERT_4_G Non-Integer Number of Atoms ( 4.20) in Resd. #  | 3     | Check  |

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

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

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

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## checkCIF publication errors

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### 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.

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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 21/04/2015; check.def file version of 09/03/2015**

