

# 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 = 0.0112 A                      Wavelength=1.54184

Cell:              a=8.2825(5)              b=9.3544(6)              c=12.0173(5)  
                    alpha=83.319(5)          beta=70.903(5)          gamma=80.102(5)

Temperature:      293 K

	Calculated	Reported
Volume	864.93(9)	864.93(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C14 H20 Mo O2 Se	?
Sum formula	C14 H20 Mo O2 Se	C14 H20 Mo O2 Se
Mr	395.20	395.20
Dx,g cm-3	1.518	1.517
Z	2	2
Mu (mm-1)	8.551	8.551
F000	392.0	392.0
F000'	390.97	
h,k,lmax	9,10,14	9,10,14
Nref	2928	5002
Tmin,Tmax	0.177,0.181	0.322,0.384
Tmin'	0.079	

Correction method= # Reported T Limits: Tmin=0.322 Tmax=0.384  
AbsCorr = MULTI-SCAN

Data completeness= 1.708                      Theta(max)= 64.984

R(reflections)= 0.0529( 4807)              wR2(reflections)= 0.1608( 5002)

S = 1.082                                      Npar= 217

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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 B**PLAT019\_ALERT\_1\_B \_diffn\_measured\_fraction\_theta\_full/\_max < 1.0 0.937 Report

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**Alert level C**

THETM01\_ALERT\_3\_C The value of sine(theta\_max)/wavelength is less than 0.590  
Calculated sin(theta\_max)/wavelength = 0.5877

PLAT048\_ALERT\_1\_C MoietyFormula Not Given ..... Please Do !  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference Mol -- C11 .. 0.16 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference O1 -- C11 .. 0.19 Ang.  
PLAT242\_ALERT\_2\_C Low Ueq as Compared to Neighbors for .... Mol Check  
PLAT242\_ALERT\_2\_C Low Ueq as Compared to Neighbors for .... C12 Check  
PLAT342\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.0112 Ang.  
PLAT480\_ALERT\_4\_C Long H...A H-Bond Reported H14A .. O2 .. 2.67 Ang.  
PLAT911\_ALERT\_3\_C Missing # FCF Refl Between THmin & STh/L= 0.588 19 Report  
PLAT918\_ALERT\_3\_C Reflection(s) with I(obs) much smaller I(calc) . 1 Check

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**Alert level G**

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 6 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report  
PLAT021\_ALERT\_4\_G Ratio Unique / Expected Reflections too High ... 1.708  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large. 0.11 Report  
PLAT154\_ALERT\_1\_G The su's on the Cell Angles are Equal ..... 0.00500 Degree  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 1 Report  
PLAT176\_ALERT\_4\_G The CIF-Embedded .res File Contains SADI Records 2 Report  
PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 3 Report  
PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check  
PLAT200\_ALERT\_1\_G Reported \_diffn\_ambient\_temperature ..... (K) 293 Check  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Mol -- Sel .. 5.2 su  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of >Sel is Constrained at 0.536 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of <Sel' is Constrained at 0.464 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of >O1 is Constrained at 0.536 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of <O1' is Constrained at 0.464 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of >C11 is Constrained at 0.536 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of >C13 is Constrained at 0.536 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of >C14 is Constrained at 0.536 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of <C11' is Constrained at 0.464 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of <C13' is Constrained at 0.464 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of <C14' is Constrained at 0.464 Check  
PLAT301\_ALERT\_3\_G Main Residue Disorder ..... Percentage = 28 Note  
PLAT811\_ALERT\_5\_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 46 Note  
PLAT909\_ALERT\_3\_G Percentage of Observed Data at Theta(Max) still 89 %

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
6 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  
17 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
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;
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 29/01/2015; check.def file version of 29/01/2015**

