

# 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 = 0.0064 A                      Wavelength=1.34180

Cell:              a=15.2868(3)              b=15.4435(3)              c=18.0918(4)  
                    alpha=100.050(1)      beta=113.033(1)      gamma=102.490(1)

Temperature:    170 K

|                | Calculated              | Reported     |
|----------------|-------------------------|--------------|
| Volume         | 3674.57(14)             | 3674.56(13)  |
| Space group    | P 1                     | P 1          |
| Hall group     | P 1                     | P 1          |
| Moiety formula | C42 H70 O35 [+ solvent] | ?            |
| Sum formula    | C42 H70 O35 [+ solvent] | C84 H140 O70 |
| Mr             | 1134.98                 | 2269.95      |
| Dx,g cm-3      | 1.026                   | 1.026        |
| Z              | 2                       | 1            |
| Mu (mm-1)      | 0.501                   | 0.504        |
| F000           | 1204.0                  | 1204.0       |
| F000'          | 1207.76                 |              |
| h,k,lmax       | 19,19,22                | 19,19,22     |
| Nref           | 30126[ 15063]           | 27008        |
| Tmin,Tmax      | 0.860,0.895             | 0.860,0.895  |
| Tmin'          | 0.860                   |              |

Correction method= # Reported T Limits: Tmin=0.860 Tmax=0.895  
AbsCorr = MULTI-SCAN

Data completeness= 1.79/0.90                      Theta(max)= 57.090

R(reflections)= 0.0648( 25912)              wR2(reflections)= 0.1912( 27008)

S = 1.028                                      Npar= 1387

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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**

PLAT097\_ALERT\_2\_B Large Reported Max. (Positive) Residual Density 1.48 eA-3  
PLAT415\_ALERT\_2\_B Short Inter D-H..H-X H6A ..H24 . 1.99 Ang.  
x,l+y,z = 1\_565 Check

PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O1 --H1 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O3 --H3 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O9 --H9 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O13 --H13 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O16 --H16 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O18 --H18 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O23 --H23 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O24 --H24 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O26 --H26 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O28 --H28 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O31 --H31 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O33 --H33 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O34 --H34 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O39 --H39 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O43 --H43 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O46 --H46 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O51 --H51 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O54 --H54 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O56 --H56 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O58 --H58 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O63 --H63 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O64 --H64 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O66 --H66 . Please Check  
PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O68 --H68 . Please Check

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**Alert level C**

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

RADNW01\_ALERT\_1\_C The radiation wavelength lies outside the expected range  
for the supplied radiation type. Expected range 1.34130-1.34150  
Wavelength given = 1.34180

PLAT048\_ALERT\_1\_C MoietyFormula Not Given (or Incomplete) ..... Please Check  
PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 2.97 Report  
PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio  
PLAT220\_ALERT\_2\_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 5.1 Ratio  
PLAT220\_ALERT\_2\_C NonSolvent Resd 2 O Ueq(max)/Ueq(min) Range 3.8 Ratio  
PLAT222\_ALERT\_3\_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.7 Ratio  
PLAT222\_ALERT\_3\_C NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range 4.3 Ratio  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference O31 --C37 . 0.18 Ang.  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C73 Check  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00636 Ang.  
PLAT415\_ALERT\_2\_C Short Inter D-H..H-X H54 ..H84A . 2.08 Ang.  
1+x,y,z = 1\_655 Check

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**Alert level G**

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 2 Note  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 42 Report  
PLAT033\_ALERT\_4\_G Flack x Value Deviates > 3.0 \* sigma from Zero . 0.260 Note  
PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 2.00 Check  
PLAT066\_ALERT\_1\_G Predicted and Reported Tmin&Tmax Range Identical ? Check  
PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 1 Report  
PLAT606\_ALERT\_4\_G Solvent Accessible VOID(S) in Structure ..... ! Info



|  |               |              |
|--|---------------|--------------|
| PLAT791_ALERT_4_G Model has Chirality at C74                       | (Sohnke SpGr) | R Verify     |
| PLAT791_ALERT_4_G Model has Chirality at C75                       | (Sohnke SpGr) | S Verify     |
| PLAT791_ALERT_4_G Model has Chirality at C76                       | (Sohnke SpGr) | R Verify     |
| PLAT791_ALERT_4_G Model has Chirality at C77                       | (Sohnke SpGr) | R Verify     |
| PLAT791_ALERT_4_G Model has Chirality at C78                       | (Sohnke SpGr) | R Verify     |
| PLAT791_ALERT_4_G Model has Chirality at C80                       | (Sohnke SpGr) | R Verify     |
| PLAT791_ALERT_4_G Model has Chirality at C81                       | (Sohnke SpGr) | S Verify     |
| PLAT791_ALERT_4_G Model has Chirality at C82                       | (Sohnke SpGr) | R Verify     |
| PLAT791_ALERT_4_G Model has Chirality at C83                       | (Sohnke SpGr) | R Verify     |
| PLAT791_ALERT_4_G Model has Chirality at C84                       | (Sohnke SpGr) | R Verify     |
| PLAT860_ALERT_3_G Number of Least-Squares Restraints .....         |               | 4 Note       |
| PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed  |               | ! Info       |
| PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . |               | Please Do !  |
| PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....       |               | 3.1 Low      |
| PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged |               | Please Check |
| PLAT984_ALERT_1_G The C-f' = 0.0150 Deviates from the B&C-Value    |               | 0.0137 Check |
| PLAT984_ALERT_1_G The O-f' = 0.0410 Deviates from the B&C-Value    |               | 0.0389 Check |

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

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
34 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  
76 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
;
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 you wish to submit your CIF for publication in IUCrData 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 22/03/2021; check.def file version of 19/03/2021**

Datablock I - ellipsoid plot

