# checkCIF () running

*Checking for embedded fcf data in CIF ...*
*No extractable fcf data in found in CIF*

# checkCIF/PLATON (full publication check)

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. You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

## Datablock: J__2017_3_5_HEXINZ~1_keti_UNDER_~1_PBTB_E~1_PBTB

Bond precision: O- B = 0.0386 A Wavelength=0.71073
Cell: a=7.7676(8) b=9.0824(10) c=13.2535(14)
alpha=90 beta=103.150(1) gamma=90
Temperature: 296 K

| | Calculated | Reported |
|---|---|---|
| Volume | 910.50(17) | 910.50(17) |
| Space group | P 21 | P 21 |
| Hall group | P 2yb | P 2yb |
| Moiety formula | B14 O26 Pb2 Tb2 | ? |
| Sum formula | B14 O26 Pb2 Tb2 | B7 O13 Pb Tb |
| Mr | 1299.60 | 649.78 |
| Dx,g cm-3 | 4.740 | 4.740 |
| Z | 2 | 4 |
| Mu (mm-1) | 26.258 | 26.258 |
| F000 | 1144.0 | 1144.0 |
| F000' | 1131.38 | |
| h,k,lmax | 10,12,17 | 10,12,17 |
| Nref | 4519[ 2401] | 4034 |
| Tmin,Tmax | 0.054,0.350 | 0.067,0.529 |
| Tmin' | 0.004 | |

Correction method= # Reported T Limits: Tmin=0.067 Tmax=0.529 AbsCorr = MULTI-SCAN
Data completeness= 1.68/0.89 Theta(max)= 28.304
R(reflections)= 0.0418( 3533) wR2(reflections)= 0.1168( 4034)
S = 1.062 Npar= 327

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 B

PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

### Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field. Absorption correction given as multi-scan

PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 7.34 Note

### Alert level G

| | | |
|---|---|---|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 2 Note |
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | 40 Report |
| PLAT004_ALERT_5_G | Polymeric Structure Found with Maximum Dimension | 3 Info |
| PLAT012_ALERT_1_G | N.O.K. _shelx_res_checksum found in CIF ..... | Please Check |
| PLAT033_ALERT_4_G | Flack x Value Deviates > 3.0 * sigma from Zero . | 0.115 Note |
| PLAT045_ALERT_1_G | Calculated and Reported Z Differ by a Factor ... | 0.50 Check |
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT Unusually Large | 7.22 Why ? |
| PLAT171_ALERT_4_G | The CIF-Embedded .res File Contains EADP Records | 13 Report |
| PLAT172_ALERT_4_G | The CIF-Embedded .res File Contains DFIX Records | 1 Report |
| PLAT186_ALERT_4_G | The CIF-Embedded .res File Contains ISOR Records | 1 Report |
| PLAT397_ALERT_2_G | Deviating B-O-B Angle from 120 Deg for O2 | 134.6 Degree |

**And 2 other PLAT397 Alerts**

| | | |
|---|---|---|
| PLAT397_ALERT_2_G | Deviating B-O-B Angle from 120 Deg for O8 | 132.8 Degree |
| PLAT397_ALERT_2_G | Deviating B-O-B Angle from 120 Deg for O13 | 133.9 Degree |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints ..... | 242 Note |
| PLAT870_ALERT_4_G | ALERTS Related to Twinning Effects Suppressed .. | ! Info |

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

4 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
2 ALERT type 3 Indicator that the structure quality may be low
5 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). |

6 **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

**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: ...
;
# 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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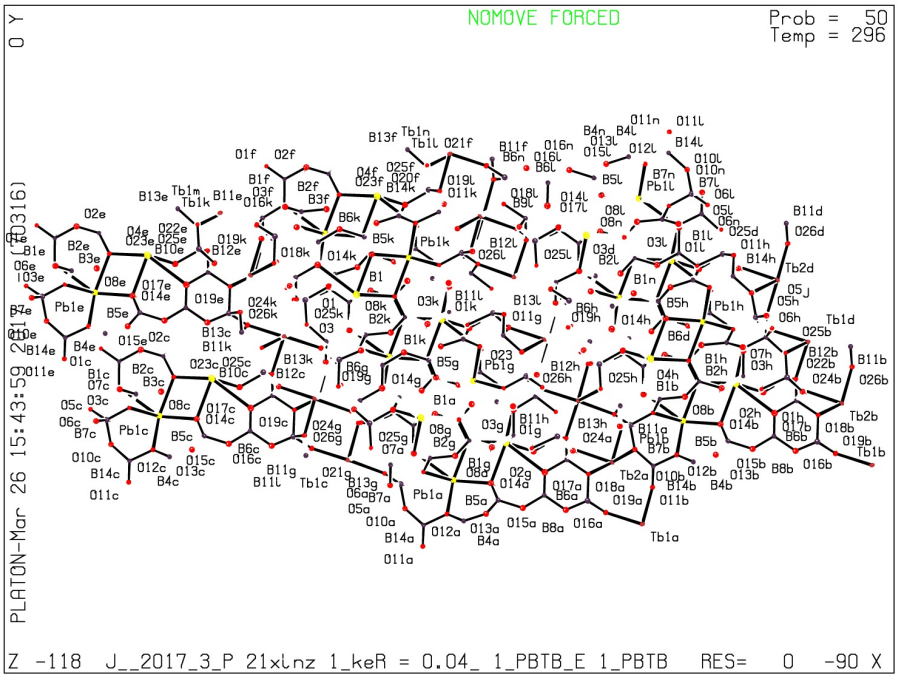
**PLATON version of 26/02/2017; check.def file version of 21/02/2017**

## Datablock J__2017_3_5_HEXINZ~1_keti_UNDER_~1_PBTB_E~1_PBTBB7~1_a - ellipsoid plot

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[Test a new CIF entry]