checkCIF () running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . .

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: I

Bond precision: O- B = 0.0318 A   Wavelength=0.71073
Cell: a=7.7988(6)   b=9.1196(7)   c=13.2883(11)
             alpha=90   beta=103.092(1) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	920.53(13)	920.52(13)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	B14 Eu2 O26 Pb2	?
Sum formula	B14 Eu2 O26 Pb2	B7 Eu O13 Pb
Mr	1285.68	642.82
Dx,g cm-3	4.639	4.638
Z	2	4
Mu (mm-1)	25.102	25.103
F000	1136.0	1136.0
F000'	1123.37	
h,k,lmax	10,12,17	10,12,17
Nref	4584[2434]	4362
Tmin,Tmax	0.015,0.285	0.157,0.482
Tmin'	0.005	

Correction method= # Reported T Limits: Tmin=0.157 Tmax=0.482 AbsCorr = MULTI-SCAN

Data completeness= 1.79/0.95   Theta(max)= 28.299

R(reflections)= 0.0349(3718)   wR2(reflections)= 0.0871(4362)

S = 1.032   Npar= 357

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
PLAT220_ALERT_2_B Non-Solvent Resd 1   B   Ueq(max)/Ueq(min) Range   9.4 Ratio
PLAT220_ALERT_2_B Non-Solvent Resd 1   O   Ueq(max)/Ueq(min) Range   6.3 Ratio
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) ........      6.82 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      2.73 Report
```

📄Alert level G

```
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 .     0.030 Note
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.50 Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         6 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  O6       134.5 Degree
```

And 2 other PLAT397 Alerts

```
PLAT397_ALERT_2_G Deviating  B-O-B  Angle from 120 Deg for  O18      130.2 Degree
PLAT397_ALERT_2_G Deviating  B-O-B  Angle from 120 Deg for  O21      137.0 Degree
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       241 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..         ! Info
```

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

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 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.
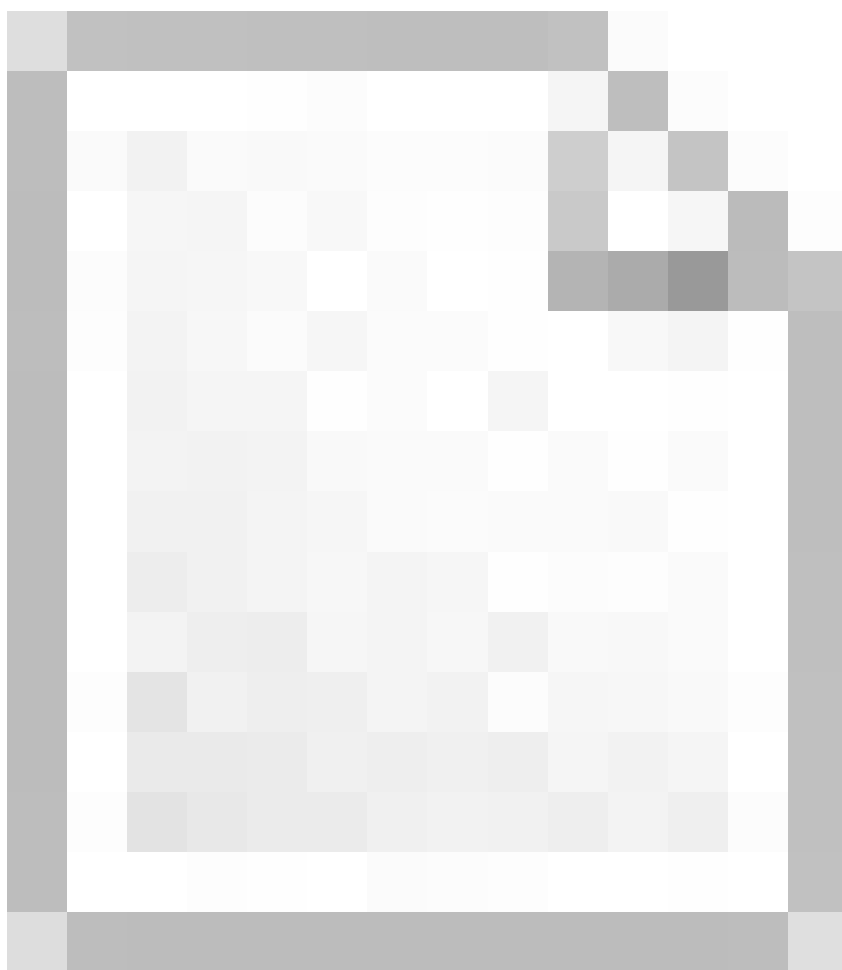
Validation response form

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 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.

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

Datablock I - ellipsoid plot

Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry