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

Bond precision: C-C = 0.0084 A   Wavelength=0.71073

| Cell: | | a=8.2128(14) | b=17.373(3) | c=10.127(2) |
| | | alpha=90 | beta=93.105(10) | gamma=90 |

Temperature: 150 K

	Calculated	Reported
Volume	1442.8(5)	1442.8(5)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C20 H17 Ca N3 O6, C12 H8 N2, H2 O	C20 H17 Ca N3 O6, C12 H8 N2, H2 O
Sum formula	C32 H27 Ca N5 O7	C32 H27 Ca N5 O7
Mr	633.67	633.67
Dx,g cm-3	1.459	1.459
Z	2	2
Mu (mm-1)	0.277	0.277
F000	660.0	660.0
F000'	660.76	
h,k,lmax	9,20,12	9,20,12
Nref	5086[2635]	5042
Tmin,Tmax	0.951,0.973	0.929,0.973
Tmin'	0.928	

Correction method= MULTI-SCAN

Data completeness= 1.91/0.99   Theta(max)= 25.020

R(reflections)= 0.0648(3917)   wR2(reflections)= 0.1554(5042)

S = 1.082   Npar= Npar = 430

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
```
PLAT415_ALERT_2_B Short Inter D-H..H-X         H3      ..   H6W     ..         2.05 Ang.
PLAT910_ALERT_3_B Missing # of FCF Reflections Below Th(Min) .....         11 Why ?
```

☄ Alert level C
```
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........         6.10 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....         3.53 Why ?
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............       0.0084 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C1      -   C2      ...       1.53 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.595            4 Why ?
PLAT975_ALERT_2_C Check Calcd Residual Density  1.05A From      O2W        0.46 eA-3
```

☄ Alert level G
```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       12 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Dimension .......        1 Info
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF    Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical        ? Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       13 Note
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) still       52 %
```

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

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

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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.

```
# 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 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 05/02/2014; check.def file version of 05/02/2014

Datablock I - ellipsoid plot