checkCIF/PLATON report

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

No syntax errors found.　　CIF dictionary　　Interpreting this report

Datablock: I

Bond precision:　C-C = 0.0053 A　　　　　Wavelength=0.71073

Cell:　　　　　a=9.2205(10)　　b=23.370(3)　　　　c=12.7620(13)
　　　　　　　　alpha=90　　　　beta=102.478(8)　　gamma=90
Temperature:　298 K

	Calculated	Reported
Volume	2685.0(5)	2685.0(5)
Space group	P 21/a	P 21/a
Hall group	-P 2yab	-P 2yab
Moiety formula	C33 H29 N3 O3	?
Sum formula	C33 H29 N3 O3	C33 H29 N3 O3
Mr	515.59	515.59
Dx,g cm-3	1.276	1.276
Z	4	4
Mu (mm-1)	0.083	0.083
F000	1088.0	1088.0
F000'	1088.45	
h,k,lmax	12,32,17	12,32,17
Nref	7375	7238
Tmin,Tmax	0.975,0.988	
Tmin'	0.967	

Correction method= Not given

Data completeness= 0.981　　　　　Theta(max)= 29.330

R(reflections)= 0.1013(3327)　　wR2(reflections)= 0.2707(7238)

S = 1.158　　　　　　　　　Npar= 352

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 C
RFACG01_ALERT_3_C　The value of the R factor is > 0.10
　　　　　R factor given　0.101
RFACR01_ALERT_3_C　The value of the weighted R factor is > 0.25
　　　　　Weighted R factor given　0.271

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given    0.125
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 .........     0.125
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low ....      46 Perc.
PLAT048_ALERT_1_C MoietyFormula Not Given ........................       ?
PLAT084_ALERT_2_C High wR2 Value .................................     0.27
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for      N2
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0053 Ang
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF        ?
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c   .......      P21/a
PLAT793_ALERT_4_G The Model has Chirality at C14     (Verify) ....        R
PLAT793_ALERT_4_G The Model has Chirality at C16     (Verify) ....        S
PLAT793_ALERT_4_G The Model has Chirality at C23     (Verify) ....        R
PLAT793_ALERT_4_G The Model has Chirality at C25     (Verify) ....        R
```

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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   9 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
   2 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

checkCIF publication errors

Alert level A

```
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.
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
           Abstract of paper in English.
```

Alert level G

```
PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is
           missing. This is required for a full paper submission (but is
           optional for an electronic paper).
PUBL017_ALERT_1_G The _publ_section_references section is missing or
           empty.
```

```
   3 ALERT level A = Data missing that is essential or data in wrong format
   2 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 Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

```
# start Validation Reply Form
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
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 05/11/2012; check.def file version of 05/11/2012