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

Bond precision: V- O = 0.0080 A Wavelength=0.71073

Cell: a=19.2623(6) b=19.2623(6) c=7.7318(2)
alpha=90 beta=90 gamma=120
Temperature: 100 K

	Calculated	Reported
Volume	2484.43(19)	2484.43(13)
Space group	P -3 m 1	P -3 m 1
Hall group	-P 3 2"	-P 3 2"
Moiety formula	2(F27 O6 V6), F27 O6 V6, Cl, 2(F), 30(K)	2(F27 O6 V6), F27 O6 V6, Cl, 2(F), 30(K)
Sum formula	Cl F83 K30 O18 V18	Cl F83 K30 O18 V18
Mr	3990.37	3990.37
Dx,g cm-3	2.667	2.667
Z	1	1
Mu (mm-1)	3.085	3.085
F000	1892.0	1892.0
F000’	1905.10	
h,k,lmax	27,27,10	27,27,10
Nref	2647	2642
Tmin,Tmax	0.648,0.691	0.333,0.709
Tmin’	0.242	

Correction method= NUMERICAL

Data completeness= 0.998 Theta(max)= 30.120

R(reflections)= 0.0613(2596) wR2(reflections)= 0.1774(2642)

S = 1.132 Npar= 139

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

```
DIFMX01_ALERT_2_B  The maximum difference density is > 0.1*ZMAX*1.00
            _refine_diff_density_max given =      2.669
            Test value =      2.300
            Crystal system given = trigonal
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       2.67 eA-3
```

Alert level C

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
            The relevant atom site should be identified.
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.05
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         V1
PLAT431_ALERT_2_C Short Inter HL..A  Contact  F5     ..  O3      .       2.85 Ang.
```

Alert level G

```
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ? Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      19.65
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...          6 Units
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ..................         14 %
PLAT434_ALERT_2_G Short Inter HL..HL Contact  F2     ..  F8      .       2.82 Ang.
PLAT794_ALERT_5_G Note: Tentative Bond Valency for V1      (V)           5.08
PLAT794_ALERT_5_G Note: Tentative Bond Valency for V3      (V)           4.94
```

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

   2 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
   0 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
```

checkCIF publication errors

Alert level A

```
PUBL002_ALERT_1_A  The contact author’s address is missing,
            _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

```
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.
```

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   7 **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

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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 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_PUBL002_GLOBAL
;
PROBLEM: The contact author’s address is 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 01/06/2013; check.def file version of 24/05/2013

Datablock I - ellipsoid plot

