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: C-C = 0.0089 A Wavelength=1.54178

Cell: a=14.8069(3) b=23.9156(5) c=15.4586(3)
alpha=90 beta=108.275(1) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	5198.03(18)	5198.03(18)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C96 H110 N8 O12, 3.17(C H Cl3)	3.17(C H Cl3), C96 H110 N8 O12
Sum formula	C99.18 H113.18 Cl9.53 N8 O12	C99.18 H113.18 Cl9.53 N8 O12
Mr	1946.92	1947.03
Dx,g cm-3	1.244	1.244
Z	2	2
Mu (mm-1)	2.826	2.827
F000	2044.3	2044.0
F000’	2056.30	
h,k,lmax	17,28,18	17,28,18
Nref	18398[9443]	16669
Tmin,Tmax	0.814,0.972	0.592,0.753
Tmin’	0.738	

Correction method= MULTI-SCAN

Data completeness= 1.77/0.91 Theta(max)= 66.606

R(reflections)= 0.0593(14262) wR2(reflections)= 0.1571(16669)

S = 1.030 Npar= Npar =1242

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

```
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.86 Why ?
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          1
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        5.4 Ratio
PLAT222_ALERT_3_C Large Non-Solvent    H    Uiso(max)/Uiso(min) ..        5.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C91    --  C93     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C91    --  C97     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C92    --  C95     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C97    --  C98     ..       0.16 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C66 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C95 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         C65 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0089 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor       N6     -   H6     ...     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N7     -   H7     ...     Please Check
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         49 Ang3
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C99.18 H113.18 Cl9.53 N8 O1
           Atom count from _chemical_formula_moiety:C99.17 H113.17 Cl9.51 N8 O1
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         22 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          8 Why ?
PLAT033_ALERT_4_G Flack x Value Deviates > 2*sigma from Zero .....      0.045
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =         84 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
             C H Cl3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4 Note
             C H Cl3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
             C H Cl3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
             C H Cl3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7 Note
             C H Cl3
PLAT791_ALERT_4_G The Model has Chirality at C45     .............          R Verify
PLAT791_ALERT_4_G The Model has Chirality at C47     .............          R Verify
PLAT791_ALERT_4_G The Model has Chirality at C48     .............          R Verify
PLAT791_ALERT_4_G The Model has Chirality at C51     .............          R Verify
PLAT791_ALERT_4_G The Model has Chirality at C52     .............          R Verify
PLAT791_ALERT_4_G The Model has Chirality at C53     .............          R Verify
PLAT791_ALERT_4_G The Model has Chirality at C58     .............          R Verify
PLAT791_ALERT_4_G The Model has Chirality at C77     .............          R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         38 Note
```

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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
  16 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  20 ALERT level G = General information/check it is not something unexpected
```

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   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  20 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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.
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   7 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.

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

Datablock I - ellipsoid plot