# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3b

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: 3b

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Bond precision:   C-C = 0.0042 A              Wavelength=0.71073

Cell:              a=7.3780(3)      b=28.1830(15)          c=14.5586(7)
                   alpha=90          beta=98.482(4)        gamma=90
Temperature:       294 K

|                | Calculated | Reported |
|----------------|------------|----------|
| Volume | 2994.1(2) | 2994.1(2) |
| Space group | P 21/n | P 1 21/n 1 |
| Hall group | -P 2yn | -P 2yn |
| Moiety formula | C24 H29 N5, 2(F6 P) | 2(F6 P), C24 H29 N5 |
| Sum formula | C24 H29 F12 N5 P2 | C24 H29 F12 N5 P2 |
| Mr | 677.46 | 677.46 |
| Dx,g cm-3 | 1.503 | 1.503 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.244 | 0.244 |
| F000 | 1384.0 | 1384.0 |
| F000' | 1385.85 | |
| h,k,lmax | 9,35,18 | 9,35,18 |
| Nref | 6124 | 6082 |
| Tmin,Tmax | 0.971,0.981 | 0.686,1.000 |
| Tmin' | 0.929 | |

Correction method= # Reported T Limits: Tmin=0.686 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.993            Theta(max)= 26.371

R(reflections)= 0.0572( 4632)      wR2(reflections)= 0.1628( 6082)

S = 1.044                   Npar= 502

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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

```
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        P1      0.138 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        P2      0.109 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C1        -C4      .       1.37 Ang.
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.00415 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   5.766 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600       21 Report
```

### Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        26 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        26 Report
PLAT012_ALERT_1_G No      _shelx_res_checksum Found in CIF ......   Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ   Please Check
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         6 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         2 Report
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        P1 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        P2 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       86% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       86% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  F12B      ..C8         2.94 Ang.
                                      1-x,1-y,1-z  =      3_666 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         2 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       648 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600        20 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         4 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         1 Info
```

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

   2 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
   5 ALERT type 3 Indicator that the structure quality may be low
   8 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.
```

```
   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.

### 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.

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## PLATON version of 18/02/2019; check.def file version of 18/02/2019

**Datablock 3b** - ellipsoid plot