# 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 = 0.0113 A Wavelength=0.71073

Cell: a=8.431(3) b=35.524(14) c=13.404(5)
alpha=90 beta=99.315(4) gamma=90
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 3962(3) | 3962(3) |
| Space group | P 21/c | P 21/c |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | 2(C36 H24 N7 O2 Ru), 2(F6 P), 2(C4 H8 O2), C H4 O | 2(C36 H24 N7 O2 Ru), 2(F6 P), 2(C4 H8 O2), C H4 O |
| Sum formula | C81 H68 F12 N14 O9 P2 Ru2 | C40.50 H34 F6 N7 O4.50 P Ru |
| Mr | 1873.57 | 936.78 |
| Dx,g cm-3 | 1.571 | 1.571 |
| Z | 2 | 4 |
| Mu (mm-1) | 0.518 | 0.518 |
| F000 | 1900.0 | 1900.0 |
| F000’ | 1896.35 | |
| h,k,lmax | 10,46,17 | 10,46,17 |
| Nref | 9083 | 9017 |
| Tmin,Tmax | 0.911,0.950 | 0.649,0.746 |
| Tmin’ | 0.902 | |

Correction method= # Reported T Limits: Tmin=0.649 Tmax=0.746
AbsCorr = EMPIRICAL

Data completeness= 0.993 Theta(max)= 27.499

R(reflections)= 0.0773( 4890) wR2(reflections)= 0.2437( 9017)

S = 1.032 Npar= 553

---

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

PLAT420_ALERT_2_B D-H Without Acceptor O5 --H45 . Please Check
PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Ru1 1.66 eA-3

---

## Alert level C

PLAT214_ALERT_2_C Atom C40 (Anion/Solvent) ADP max/min Ratio 4.3 prolat
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C37 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C39 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.6 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.3 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O3 0.113 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O5 0.176 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01131 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.485 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.44A From C41 1.52 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.68A From O5 0.94 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.99A From O5 0.73 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.05A From O5 0.61 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.94A From O5 0.45 eA-3

---

## Alert level G

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: C40.5 H34 F6 N7 O4.5 P1 Ru1
Atom count from _chemical_formula_moiety:C81 H68 F12 N14 O9 P2 Ru2
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P1 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O5 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C41 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H45 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H46 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H47 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H48 Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4 ) 100% Note
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C7 -C16 . 1.44 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact O5 ..C41 2.34 Ang.
1-x,1-y,2-z = 3_667 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C41 ..C41 1.41 Ang.
1-x,1-y,2-z = 3_667 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 188 Check
H47 -C41 -H48 1.555 1.555 3.667 29.80 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3 Note
C4 H8 O2
PLAT794_ALERT_5_G Tentative Bond Valency for Ru1 (III) . 3.05 Info

```
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        11 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        60 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       2.6 Low
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...        26 Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged    Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
```

---

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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  19 ALERT type 2 Indicator that the structure model may be wrong or deficient
   8 ALERT type 3 Indicator that the structure quality may be low
  17 ALERT type 4 Improvement, methodology, query or suggestion
   2 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.
```

---

### 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.

**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.

---

**PLATON version of 05/12/2020; check.def file version of 05/12/2020**

**Datablock I** - ellipsoid plot