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 = 0.0132 A              Wavelength=0.71073

Cell:          a=12.7611(11)      b=13.4218(12)      c=13.7488(13)
               alpha=63.102(1)    beta=84.443(3)    gamma=71.574(2)
Temperature:   293 K

                   Calculated                 Reported
Volume             1989.5(3)                  1989.5(3)
Space group        P -1                       P-1
Hall group         -P 1                       ?
                   C78 H70 N4 O12 Pr2 [+
Moiety formula                                ?
                   solvent]
                   C78 H70 N4 O12 Pr2 [+
Sum formula                                   C39 H35 N2 O6 Pr
                   solvent]
Mr                 1537.20                    768.60
Dx,g cm-3          1.283                      1.283
Z                  1                          2
Mu (mm-1)          1.267                      1.267
F000               780.0                      780.0
F000'              779.86
h,k,lmax           15,15,16                   15,15,16
Nref               7021                       6913
Tmin,Tmax          0.808,0.870                0.777,0.873
Tmin'              0.766

Correction method= # Reported T Limits: Tmin=0.777 Tmax=0.873
AbsCorr = MULTI-SCAN

Data completeness= 0.985          Theta(max)= 25.020

R(reflections)= 0.0500( 5536)     wR2(reflections)= 0.1241( 6913)

S = 1.064                    Npar= 433
```

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
PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE Job ...   ! Note

---

Alert level C
PLAT048_ALERT_1_C MoietyFormula Not Given (or Incomplete) ....   Please Check
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given .....   Please Do !
PLAT199_ALERT_1_C Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_C Reported   _diffrn_ambient_temperature ..... (K)   293 Check
PLAT220_ALERT_2_C NonSolvent   Resd 1 C   Ueq(max)/Ueq(min) Range   3.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C7   --C9   .   0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C14   --C15   .   0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C22   --C23   .   0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C23   --C24   .   0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C25   --C27   .   0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   O2 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   O5 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C5 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C14 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C22 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C24 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   Pr1 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C7 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.01315 Ang.

Alert level G
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF   Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.50 Check
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as   mixed Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ....   ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pr1   (III)   .   3.24 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed   ! Info
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL/   2018 Note

---

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

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   9 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 22/03/2021; check.def file version of 19/03/2021