checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a

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: a

Bond precision: C-C = 0.0053 A   Wavelength=0.71073

Cell: a=12.428(9)   b=14.064(10)   c=25.185(18)
               alpha=90   beta=101.955(9)   gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	4307(5)	4307(5)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C54 H36 N4 O, 2(C H4 O)	C54 H36 N4 O, 2(C H4 O)
Sum formula	C56 H44 N4 O3	C56 H44 N4 O3
Mr	820.95	820.95
Dx,g cm-3	1.266	1.266
Z	4	4
Mu (mm-1)	0.079	0.079
F000	1728.0	1728.0
F000'	1728.68	
h,k,lmax	15,17,30	15,15,30
Nref	8010	7678
Tmin,Tmax	0.986,0.989	0.568,0.746
Tmin'	0.986	

Correction method= # Reported T Limits: Tmin=0.568 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.959   Theta(max)= 25.500

R(reflections)= 0.0734(4430)   wR2(reflections)= 0.2359(7678)

S = 1.047   Npar= 572

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

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
            The relevant atom site should be identified.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.960 Why?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      2.25 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density      0.61 eA-3
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C1       --C6      .        6.0 s.u.
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O2     0.103 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O3     0.144 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.00528 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X       H3A      ..H56C           1.99 Ang.
                                        x,y,z  =     1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   11.889 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......    2.399 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600      243 Report
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Alert level G

```
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 ..............       2 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large    0.13 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records       1 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       1 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       6 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       3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...       4 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........     3.4 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ       2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ       2 Units
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......  Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       1 Info
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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
  12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

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_DIFMX02_a
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT029_a
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .     0.960 Why?
RESPONSE: ...
```

```
;
_vrf_PLAT094_a
;
PROBLEM: Ratio of Maximum / Minimum Residual Density ....      2.25 Report
RESPONSE: ...
;
_vrf_PLAT097_a
;
PROBLEM: Large Reported Max.  (Positive) Residual Density     0.61 eA-3
RESPONSE: ...
;
_vrf_PLAT230_a
;
PROBLEM: Hirshfeld Test Diff for     C1        --C6        .       6.0 s.u.
RESPONSE: ...
;
_vrf_PLAT260_a
;
PROBLEM: Large Average Ueq of Residue Including       O2     0.103 Check
RESPONSE: ...
;
_vrf_PLAT340_a
;
PROBLEM: Low Bond Precision on  C-C Bonds ...............   0.00528 Ang.
RESPONSE: ...
;
_vrf_PLAT414_a
;
PROBLEM: Short Intra D-H..H-X       H3A      ..H56C           1.99 Ang.
RESPONSE: ...
;
_vrf_PLAT906_a
;
PROBLEM: Large K Value in the Analysis of Variance ......   11.889 Check
RESPONSE: ...
;
_vrf_PLAT911_a
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600        243 Report
RESPONSE: ...
;
# end Validation Reply Form
```

It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 10/08/2020; check.def file version of 06/08/2020

NOMOVE FORCED

Prob = 50
Temp = 296

-38 Y

PLATON-Aug 27 12:50:15 2020 — (100820)

Z -163 a   P 1 21/c 1   R = 0.07   RES= 0-122 X