checkCIF/PLATON report

No syntax errors found.　　　**CIF dictionary**　　　**Interpreting this report**

Datablock: ud0534_2

Bond precision:　　C-C = 0.0034 A　　　　　Wavelength=0.71073

Cell:　　　　　　a=10.2623(5)　　b=11.3590(6)　　c=14.7950(8)
　　　　　　　　alpha=90　　　　beta=90　　　　gamma=90
Temperature:　　100 K

	Calculated	Reported
Volume	1724.65(16)	1724.65(16)
Space group	P 21 21 21	P2(1)2(1)2(
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C15 H9 O2, C5 H10 N3	C15 H9 O2, C5 H10 N3
Sum formula	C20 H19 N3 O2	C20 H19 N3 O2
Mr	333.38	333.38
Dx,g cm-3	1.284	1.284
Z	4	4
Mu (mm-1)	0.085	0.085
F000	704.0	704.0
F000'	704.28	
h,k,lmax	14,16,21	14,15,21
Nref	3158[5614]	3088
Tmin,Tmax	0.972,0.996	0.972,0.996
Tmin'	0.955	

Correction method= MULTI-SCAN

Data completeness= 0.98/0.55　　　Theta(max)= 31.230

R(reflections)= 0.0440(2488)　　wR2(reflections)= 0.1478(3088)

S = 1.076　　　　　　　Npar= 231

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
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low ....　　0.98
PLAT230_ALERT_2_C Hirshfeld Test Diff for　　C14　　-- C15　　..　　5.33 su
PLAT241_ALERT_2_C Check High　　Ueq as Compared to Neighbors for　　C14

⚪ Alert level G

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REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
                correct. If it is not, please give the correct count in the
                _publ_section_exptl_refinement section of the submitted CIF.
            From the CIF: _diffrn_reflns_theta_max            31.23
            From the CIF: _reflns_number_total               3088
            Count of symmetry unique reflns          3158
            Completeness (_total/calc)             97.78%
            TEST3: Check Friedels for noncentro structure
            Estimate of Friedel pairs measured            0
            Fraction of Friedel pairs measured       0.000
            Are heavy atom types Z>Si present            no
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....            ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max    datum ....            ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min    datum ....            ?
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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
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   4 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 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
   1 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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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*, 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 24/03/2011; check.def file version of 16/03/2011