## checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

## Datablock: s92

Bond precision:	C-C = 0.0033 A	Wavelength=0.71073	
Cell:	a=18.5858(10) alpha=90		c=8.0285(4) gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	1141.35(9)	1141.35(9)	)
Space group	P 21 21 2	P21212	
Hall group	P 2 2ab	?	
Moiety formula	C5 H8 N O3, C4 H12 N	I ?	
Sum formula	C9 H20 N2 O3	C9 H20 N2	03
Mr	204.27	204.27	
Dx,g cm-3	1.189	1.189	
Z	4	4	
Mu (mm-1)	0.089	0.089	
F000	448.0	448.0	
F000'	448.21		
h,k,lmax	22,9,9	22,9,9	
Nref	1228( 2071)	1217	
Tmin,Tmax	0.991,0.997	0.989,0.99	94
Tmin'	0.991		
Correction method= AbsCorr=MULTI-SCAN			
Data completeness= 0.99(0.59) Theta(max)= 25.210			
R(reflections)= 0.0385( 982) wR2(reflections)= 0.0970( 1217)			
S = 1.052 Npar= 138			

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 G

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 25.21
 From the CIF: \_reflns\_number\_total 1217
 Count of symmetry unique reflns 1228

```
Completeness (_total/calc)99.10%TEST3: Check Friedels for noncentro structureEstimate of Friedel pairs measured0Fraction of Friedel pairs measured0.000Are heavy atom types Z>Si presentnoPLAT791_ALERT_1_G Confirm the Absolute Configuration of C3...RPLAT860_ALERT_3_G Note: Number of Least-Squares Restraints1
```

```
0 ALERT level A = In general: serious problem
0 ALERT level B = Potentially serious problem
0 ALERT level C = Check and explain
3 ALERT level G = General alerts; check
1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
```

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 27/11/2007; check.def file version of 27/11/2007

Datablock s92 - ellipsoid plot

