

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) fs256a_0m

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: fs256a_0m

Bond precision: = 0.0000 A Wavelength=0.71073

Cell: a=7.4604(2) b=13.2359(4) c=9.7659(3)
 alpha=90 beta=107.814(2) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	918.10(5)	918.10(5)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C11 H10 N2 O	C11 H10 N2 O
Sum formula	C11 H10 N2 O	C11 H10 N2 O
Mr	186.21	186.21
Dx,g cm-3	1.347	1.347
Z	4	4
Mu (mm-1)	0.089	0.089
F000	392.0	392.0
F000'	392.15	
h,k,lmax	9,17,12	9,17,12
Nref	4257[2221]	2213
Tmin,Tmax	0.970,0.983	0.947,0.983
Tmin'	0.955	

Correction method= MULTI-SCAN

Data completeness= 1.00/0.52 Theta(max)= 27.580

R(reflections)= 0.0429(1456) wR2(reflections)= 0.1358(2213)

S = 1.130 Npar= 362

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

PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18)	6.11
PLAT165_ALERT_3_C	Nr. of Status R Flagged Non-Hydrogen Atoms	4
PLAT213_ALERT_2_C	Atom O1A has ADP max/min Ratio	3.6 prola
PLAT213_ALERT_2_C	Atom O1B has ADP max/min Ratio	3.6 prola
PLAT213_ALERT_2_C	Atom C5B has ADP max/min Ratio	3.3 prola
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.2

● Alert level G

PLAT230_ALERT_2_G	Hirshfeld Test Diff for C2A -- C9A ..	5.8 su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C10A -- C11A ..	5.6 su
PLAT242_ALERT_2_G	Check Low Ueq as Compared to Neighbors for C9A	
PLAT242_ALERT_2_G	Check Low Ueq as Compared to Neighbors for C5Y	
PLAT301_ALERT_3_G	Note: Main Residue Disorder	100 %
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C3Y -C8Y	0.22 Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	28
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	7

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

0 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
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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.

