

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 241112zyd_3_muban

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: 241112zyd_3_muban

Bond precision:	C-C = 0.0066 A	Wavelength=0.71073		
Cell:	a=6.1503 (2)	b=16.9911 (7)	c=20.2854 (8)	
	alpha=90	beta=90	gamma=90	
Temperature:	296 K			

	Calculated	Reported
Volume	2119.83(14)	2119.83(14)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C24 H25 N O S	C24 H25 N O S
Sum formula	C24 H25 N O S	C24 H25 N O S
Mr	375.51	375.51
Dx, g cm ⁻³	1.177	1.177
Z	4	4
Mu (mm ⁻¹)	0.165	0.165
F000	800.0	800.0
F000'	800.78	
h, k, lmax	7, 22, 26	7, 22, 26
Nref	4849[2789]	4822
Tmin, Tmax	0.972, 0.992	0.682, 0.746
Tmin'	0.972	

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Correction method= # Reported T Limits: Tmin=0.682 Tmax=0.746
AbsCorr = MULTI-SCAN
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Data completeness= 1.73/0.99 Theta(max)= 27.477

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R(reflections)= 0.0604( 3025)      wR2(reflections)=
S = 1.034                        0.1409( 4822)
Npar= 278
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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

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C11	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C14	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C18	Check
PLAT340_ALERT_3_C	Low	Bond Precision on C-C Bonds	0.00662	Ang.
PLAT906_ALERT_3_C	Large	K Value in the Analysis of Variance	3.474	Check
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L= 0.600	5	Report
		1 2 1, 1 0 2, 0 3 2, 0 4 2, 0 3 3,		
PLAT913_ALERT_3_C	Missing	# of Very Strong Reflections in FCF	5	Note
		1 2 1, 1 0 2, 0 3 2, 0 4 2, 0 3 3,		



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7	Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H Atoms	7	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	11%	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	75	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4	Note
	0 2 0, 0 1 1, 0 0 2, 0 1 2,		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3	Note
	0 0 2, 0 1 1, 0 1 2,		
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	2.788	Note
	Predicted wR2: Based on SigI**2 5.05 or SHELX Weight 13.63		
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
1 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* 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.

