



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2971_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: 2971_a

Bond precision:	C-C = 0.0017 Å	Wavelength=0.71073
Cell:	a=11.9241 (3) alpha=90	b=16.2376 (4) beta=95.505 (1)
Temperature:	100 K	c=7.1175 (2) gamma=90
	Calculated	Reported
Volume	1371.73 (6)	1371.73 (6)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C15 H12 O5 S	?
Sum formula	C15 H12 O5 S	C15 H12 O5 S
Mr	304.31	304.31
Dx, g cm ⁻³	1.474	1.474
Z	4	4
Mu (mm ⁻¹)	0.255	0.255
F000	632.0	632.0
F000'	632.85	
h, k, lmax	15, 21, 9	15, 21, 9
Nref	3417	3400
Tmin, Tmax	0.964, 0.976	0.955, 0.976
Tmin'	0.954	

Correction method= # Reported T Limits: Tmin=0.955 Tmax=0.976
AbsCorr = MULTI-SCAN

Data completeness= 0.995

Theta(max)= 28.319

R(reflections)= 0.0394(3094)

wR2(reflections)=
0.1418(3400)

S = 1.202

Npar= 192

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

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.42 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 6 Report
1 2 0, 0 6 0, 4 1 1, 3 4 2, -2 5 2, 3 9 3,



Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]= 2.13 Note
1 0 0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 10 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 6 Note
3 9 3, 1 2 0, 0 6 0, 4 1 1, 3 4 2, -2 5 2,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 5.294 Note
Predicted wR2: Based on SigI**2 2.68 or SHELX Weight 11.80 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 13 Info

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 23/04/2026; check.def file version of 30/03/2026

duplicate check

No duplication found

Datablock 2971_a - ellipsoid plot

