



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) A26002_002

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: A26002_002

Bond precision: C-C = 0.0038 Å

Wavelength=0.71073

Cell: a=9.270 (2) b=10.189 (3) c=10.794 (3)
 alpha=95.896 (9) beta=108.539 (8) gamma=93.433 (9)
Temperature: 296 K

	Calculated	Reported
Volume	956.9 (4)	956.9 (5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C19 H14 Cl2 N2 O3 S	C19 H14 Cl2 N2 O3 S
Sum formula	C19 H14 Cl2 N2 O3 S	C19 H14 Cl2 N2 O3 S
Mr	421.28	421.28
Dx, g cm ⁻³	1.462	1.462
Z	2	2
Mu (mm ⁻¹)	0.471	0.471
F000	432.0	432.0
F000'	433.00	
h, k, lmax	11, 12, 13	11, 12, 13
Nref	3786	3775
Tmin, Tmax	0.984, 0.987	0.708, 0.745
Tmin'	0.975	

Correction method= # Reported T Limits: Tmin=0.708 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.997

Theta(max)= 26.029

R(reflections)= 0.0449(2838)

wR2(reflections)=
0.0996(3775)

S = 1.085

Npar= 248

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

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 6.136 Check



Alert level G

PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]= 2.53 Note
1 0 0, 0 1 0, 0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 7 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.041 Note
Predicted wR2: Based on SigI**2 3.28 or SHELX Weight 9.18
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **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
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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 26/09/2025; check.def file version of 20/09/2025

