



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CEC0532_1

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: CEC0532_1

Bond precision: C-C = 0.0023 Å

Wavelength=0.71073

Cell: a=14.6094 (4) b=5.9626 (2) c=28.8704 (8)

 alpha=90

 beta=90

 gamma=90

Temperature: 85 K

	Calculated	Reported
Volume	2514.90 (13)	2514.90 (13)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C14 H17 N O S	C14 H17 N O S
Sum formula	C14 H17 N O S	C14 H17 N O S
Mr	247.35	247.34
Dx, g cm ⁻³	1.307	1.307
Z	8	8
Mu (mm ⁻¹)	0.240	0.240
F000	1056.0	1056.0
F000'	1057.35	
h, k, lmax	24, 9, 48	24, 9, 48
Nref	12236 [6215]	12223
Tmin, Tmax	0.974, 0.980	0.910, 0.980
Tmin'	0.967	

Correction method= # Reported T Limits: Tmin=0.910 Tmax=0.980
AbsCorr = MULTI-SCAN

Data completeness= 1.97/1.00 Theta(max)= 36.370

R(reflections)= 0.0421(12050)

wR2(reflections)=
0.1141(12223)

S = 1.152

Npar= 324

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 B

PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density 4.84 Report

Author Response: The thiophen rings are very slightly disordered by a 180 deg rotation which gives rise to two moderate density peaks of the disordered positions of the sulfurs in the two independent mols. These two peaks stick out from the density map.

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 1.63 eA-3

Author Response: The thiophen rings are very slightly disordered by a 180 deg rotation giving rise to two moderate density peaks of the disordered positions of the sulfurs in the two independent mols.

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

STRVA01_ALERT_4_C Flack test results are ambiguous.

From the CIF: _refine_ls_abs_structure_Flack 0.690

From the CIF: _refine_ls_abs_structure_Flack_su 0.050

PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N9	--H9A	.	Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N9	--H9B	.	Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N29	--H29A	.	Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N29	--H29B	.	Please Check
PLAT907_ALERT_2_C	Flack x > 0.5, Structure Needs to be Inverted?	.		0.69	Check
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.83Ang From N29	.	0.51	eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
	H17 H37		
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0100	Report
PLAT792_ALERT_1_G	Model has Chirality at C6	(Polar SpGr)	S Verify
PLAT792_ALERT_1_G	Model has Chirality at C8	(Polar SpGr)	S Verify
PLAT792_ALERT_1_G	Model has Chirality at C26	(Polar SpGr)	R Verify

PLAT792_ALERT_1_G	Model has Chirality at C28	(Polar SpGr)	R Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		7 Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta (Min) [Deg]=		2.79 Note
	0 0 2,		
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		1 Note
	4 0 9,		
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..		73.0 Degree
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		6.372 Note
	Predicted wR2: Based on SigI**2 1.79 or SHELX Weight	9.90	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		8 Info

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 11 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
 3 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. 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

