

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: _143628_2

Bond precision: C-C = 0.0030 Å

Wavelength=1.54187

Cell: a=7.4367(4) b=8.3023(4) c=12.3159(7)
 alpha=100.874(3) beta=104.217(3) gamma=109.047(3)
Temperature: 293 K

	Calculated	Reported
Volume	666.11(7)	666.11(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C14 H15 N3 O2 S	C14 H15 N3 O2 S
Sum formula	C14 H15 N3 O2 S	C14 H15 N3 O2 S
Mr	289.35	289.35
Dx, g cm ⁻³	1.443	1.443
Z	2	2
Mu (mm ⁻¹)	2.211	2.212
F000	304.0	304.0
F000'	305.50	
h,k,lmax	9,10,15	9,10,15
Nref	2599	2268
Tmin,Tmax	0.617,0.784	0.637,0.781
Tmin'	0.480	

Correction method= # Reported T Limits: Tmin=0.637 Tmax=0.781
AbsCorr = MULTI-SCAN

Data completeness= 0.873

Theta(max)= 71.550

R(reflections)= 0.0330(4107)

wR2(reflections)=
0.0530(4139)

S = 1.025

Npar= 241

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 A

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.873 Why?

Author Response: Although some large-theta reflexions are too weak but there is no doubt about the chemical structure taking into account other evidences, e.g. NMR. The error maybe due to crystal imperfections.

PLAT733_ALERT_1_A Torsion Calc -179.9(3), Rep -180.00(2) 9.90 s.u.-R
C(10-C(9)-C(11-C(15 1_555 1_555 1_555 1_555 # 33 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

Alert level B

REFLT02_ALERT_1_B The number of reflections greater than the sigma threshold
cannot exceed the number of symmetry-independent reflections
Number of symmetry-independent reflections = 2268
Number of reflections greater than sigma threshold = 4107

PLAT230_ALERT_2_B Hirshfeld Test Diff for S1 --O2 . 11.8 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for S1 --O3 . 8.4 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for S1 --N5 . 10.0 s.u.

Alert level C

PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H1 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H2 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H3 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H4 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H5 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H6 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H7 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H8 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H9 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H10 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H11 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H12 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H13 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H14 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H15 Note
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 6.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C8 --C13 . 6.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C11 --C15 . 5.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C15 --C18 . 5.7 s.u.
PLAT245_ALERT_2_C U(iso) H1 Smaller than U(eq) N4 by 0.011 Ang**2
PLAT703_ALERT_1_C Torsion Calc -57.72(16), Rep -57.9(2), Dev.. 1.13 Sigma

O(2)-S(1)-N(5)-N(6)	1_555	1_555	1_555	1_555	#	1 Check
PLAT703_ALERT_1_C Torsion Calc	-55.7(2), Rep	-55.4(3), Dev..				1.50 Sigma
O(3)-S(1)-N(5)-C(20)	1_555	1_555	1_555	1_555	#	6 Check
PLAT703_ALERT_1_C Torsion Calc	-170.8(2), Rep	-170.5(3), Dev..				1.50 Sigma
C(7)-S(1)-N(5)-C(20)	1_555	1_555	1_555	1_555	#	12 Check
PLAT703_ALERT_1_C Torsion Calc	-178.1(2), Rep	-178.5(3), Dev..				2.00 Sigma
C(20)-N(5)-N(6)-C(8)	1_555	1_555	1_555	1_555	#	18 Check

Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found	in the CIF	Please Do !
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..	(Note)	0.003 Degree
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	(K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	(K)	293 Check
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT882_ALERT_1_G	No Datum for _diffrn_reflns_av_unetI/netI		Please Do !
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !

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- 2 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 4 **ALERT level B** = A potentially serious problem, consider carefully
 - 24 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 - 7 **ALERT level G** = General information/check it is not something unexpected
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- 11 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
 - 2 ALERT type 3 Indicator that the structure quality may be low
 - 15 ALERT type 4 Improvement, methodology, query or suggestion
 - 2 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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_REFLT02__143628_2
;
PROBLEM: The number of reflections greater than the sigma threshold
RESPONSE: ...
;
_vrf_PLAT230__143628_2
;
PROBLEM: Hirshfeld Test Diff for      S1          --O2          .          11.8 s.u.
RESPONSE: ...
;
_vrf_PLAT166__143628_2
;
PROBLEM: S.U's Given on Coordinates for Calc-flagged ....          H1 Note
RESPONSE: ...
;
_vrf_PLAT222__143628_2
;
PROBLEM: NonSolvent Resd 1   H   Uiso(max)/Uiso(min) Range          6.3 Ratio
RESPONSE: ...
;
_vrf_PLAT245__143628_2
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;
PROBLEM: U(iso) H1          Smaller than U(eq) N4          by          0.011 Ang**2
RESPONSE: ...
;
_vrf_PLAT703__143628_2
;
PROBLEM: Torsion Calc  -57.72(16), Rep    -57.9(2), Dev..          1.13 Sigma
RESPONSE: ...
;
# end Validation Reply Form

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PLATON version of 02/02/2025; check.def file version of 02/02/2025

Datablock _143628_2 - ellipsoid plot

