

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: 142611 1

Bond precision:	C-C = 0.0023 A	Wavelength=1.54187	
Cell:	a=7.6009 (5)	b=17.131 (1)	c=10.9012 (8)
	alpha=90	beta=95.705 (4)	gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	1412.43(16)	1412.43(16)
Space group	P 21/a	P 1 21/a 1
Hall group	-P 2yab	-P 2yab
Moiety formula	C14 H17 N3 O2 S	C14 H17 N3 O2 S
Sum formula	C14 H17 N3 O2 S	C14 H17 N3 O2 S
Mr	291.37	291.37
Dx, g cm ⁻³	1.370	1.370
Z	4	4
Mu (mm ⁻¹)	2.086	2.086
F000	616.0	616.0
F000'	619.00	
h, k, lmax	9, 21, 13	9, 21, 12
Nref	2745	2587
Tmin, Tmax	0.669, 0.882	0.605, 0.882
Tmin'	0.251	

```
Correction method= # Reported T Limits: Tmin=0.605 Tmax=0.882
AbsCorr = MULTI-SCAN
```

Data completeness= 0.942 Theta (max)= 71.390

R(reflections)= 0.0510(9521)	wR2(reflections)= 0.0706(9573)
S = 1.119	Npar= 204

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

DIFMN02_ALERT_2_A The minimum difference density is $< -0.1 \times Z_{\text{MAX}} \times 2.00$
_refine_diff_density_min given = -4.410
Test value = -3.200

Author Response: Although the residual density is out of border but there is no doubt about the chemical structure taking into account other evidences, e.g. NMR. The error maybe due to crystal imperfections.

PLAT097_ALERT_2_A Large Reported Max. (Positive) Residual Density 5.84 eA-3

Author Response: Although the residual density is out of border but there is no doubt about the chemical structure taking into account other evidences, e.g. NMR. The error maybe due to crystal imperfections.

PLAT098_ALERT_2_A Large Reported Min. (Negative) Residual Density -4.41 eA-3

Author Response: Although the residual density is out of border but there is no doubt about the chemical structure taking into account other evidences, e.g. NMR. The error maybe due to crystal imperfections.

PLAT703_ALERT_1_A Torsion Calc 176.52(12), Rep 176.9(2), Dev.. 3.17 Sigma
N(6)-N(5)-C(16)-C(17 1_555 1_555 1_555 1_555 # 18 Check

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

PLAT703_ALERT_1_A Torsion Calc -174.83(13), Rep -174.3(2), Dev.. 4.08 Sigma
C(16)-N(5)-N(6)-C(19 1_555 1_555 1_555 1_555 # 20 Check

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

PLAT703_ALERT_1_A Torsion Calc -176.32(12), Rep -176.8(2), Dev.. 4.00 Sigma
C(10)-C(7)-C(15)-S(1) 1_555 1_555 1_555 1_555 # 25 Check

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

PLAT703_ALERT_1_A Torsion Calc 165.75(14), Rep 164.9(2), Dev.. 6.07 Sigma
C(15-C(11-C(16-C(17 1_555 1_555 1_555 1_555 # 43 Check

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

PLAT703_ALERT_1_A Torsion Calc 69.09(19), Rep 69.9(3), Dev.. 4.26 Sigma
C(20-C(14-C(18-N(4) 1_555 1_555 1_555 1_555 # 50 Check

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

PLAT703_ALERT_1_A Torsion Calc -108.8(2), Rep -107.6(3), Dev.. 6.00 Sigma
C(20-C(14-C(18-C(12 1_555 1_555 1_555 1_555 # 51 Check

Author Response: The structre 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 = 2587
Number of reflections greater than sigma threshold = 9521
PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low . 0.942 Why?
PLAT230_ALERT_2_B Hirshfeld Test Diff for S1 --O2 . 9.1 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for S1 --O3 . 9.9 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for S1 --N6 . 7.3 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C7 --C15 . 9.2 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C12 --C13 . 9.5 s.u.
PLAT703_ALERT_1_B Torsion Calc 150.26(12), Rep 149.9(2), Dev.. 3.00 Sigma
O(3)-S(1)-C(15-C(11 1_555 1_555 1_555 1_555 # 8 Check

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

PLAT703_ALERT_1_B Torsion Calc 0.58(18), Rep 0.2(2), Dev.. 2.11 Sigma
C(7)-N(4)-C(18-C(12 1_555 1_555 1_555 1_555 # 13 Check

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

PLAT703_ALERT_1_B Torsion Calc -0.57(17), Rep -0.1(2), Dev.. 2.76 Sigma
C(18-N(4)-C(7)-C(10 1_555 1_555 1_555 1_555 # 15 Check

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

PLAT703_ALERT_1_B Torsion Calc -179.61(16), Rep -179.2(2), Dev.. 2.56 Sigma
N(4)-C(7)-C(15-C(11 1_555 1_555 1_555 1_555 # 24 Check

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

PLAT703_ALERT_1_B Torsion Calc -0.4(2), Rep 0.1(3), Dev.. 2.50 Sigma
C(15-C(7)-C(10-C(9) 1_555 1_555 1_555 1_555 # 27 Check

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

PLAT703_ALERT_1_B Torsion Calc 179.66(15), Rep -180.0(2), Dev.. 2.27 Sigma
C(15-C(7)-C(10-C(12 1_555 1_555 1_555 1_555 # 28 Check

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

PLAT703_ALERT_1_B Torsion Calc -17.8(2), Rep -18.4(4), Dev.. 3.00 Sigma
C(8)-C(11-C(16-C(17 1_555 1_555 1_555 1_555 # 41 Check

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

PLAT703_ALERT_1_B Torsion Calc -16.8(2), Rep -17.3(4), Dev.. 2.50 Sigma
C(15-C(11-C(16-N(5) 1_555 1_555 1_555 1_555 # 42 Check

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

Alert level C

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.

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

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
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for N5 --N6 . 6.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C11 --C16 . 5.5 s.u.
PLAT703_ALERT_1_C Torsion Calc 98.60(14), Rep 98.4(2), Dev.. 1.43 Sigma
O(2)-S(1)-C(15-C(7) 1_555 1_555 1_555 1_555 # 3 Check

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

PLAT703_ALERT_1_C Torsion Calc -79.05(13), Rep -79.3(2), Dev.. 1.92 Sigma
O(2)-S(1)-C(15-C(11 1_555 1_555 1_555 1_555 # 4 Check

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

PLAT703_ALERT_1_C Torsion Calc -32.08(16), Rep -32.4(2), Dev.. 2.00 Sigma
O(3)-S(1)-C(15-C(7) 1_555 1_555 1_555 1_555 # 7 Check

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

PLAT703_ALERT_1_C Torsion Calc -145.05(14), Rep -144.8(2), Dev.. 1.79 Sigma
N(6)-S(1)-C(15-C(7) 1_555 1_555 1_555 1_555 # 9 Check

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

PLAT703_ALERT_1_C Torsion Calc 37.30(14), Rep 37.5(2), Dev.. 1.43 Sigma
N(6)-S(1)-C(15-C(11 1_555 1_555 1_555 1_555 # 10 Check

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

PLAT703_ALERT_1_C Torsion Calc -56.42(12), Rep -56.6(2), Dev.. 1.50 Sigma
C(15-S(1)-N(6)-N(5) 1_555 1_555 1_555 1_555 # 11 Check

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

PLAT703_ALERT_1_C Torsion Calc 163.17(12), Rep 163.0(2), Dev.. 1.42 Sigma
C(15-S(1)-N(6)-C(19 1_555 1_555 1_555 1_555 # 12 Check

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

PLAT703_ALERT_1_C Torsion Calc -179.78(17), Rep 179.9(2), Dev.. 1.88 Sigma
C(18-N(4)-C(7)-C(15 1_555 1_555 1_555 1_555 # 16 Check

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

PLAT703_ALERT_1_C Torsion Calc 43.16(17), Rep 43.5(3), Dev.. 2.00 Sigma
C(16-N(5)-N(6)-S(1) 1_555 1_555 1_555 1_555 # 19 Check

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

PLAT703_ALERT_1_C Torsion Calc -179.73(14), Rep -179.9(2), Dev.. 1.21 Sigma
N(4)-C(7)-C(10-C(9) 1_555 1_555 1_555 1_555 # 21 Check

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

PLAT703_ALERT_1_C Torsion Calc 0.35(17), Rep 0.1(2), Dev.. 1.47 Sigma
N(4)-C(7)-C(10-C(12 1_555 1_555 1_555 1_555 # 22 Check

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

PLAT703_ALERT_1_C Torsion Calc 1.3(2), Rep 0.9(4), Dev.. 2.00 Sigma
C(10-C(7)-C(15-C(11 1_555 1_555 1_555 1_555 # 26 Check

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

PLAT703_ALERT_1_C Torsion Calc -0.1(2), Rep -0.4(4), Dev.. 1.50 Sigma
C(8)-C(9)-C(10-C(7) 1_555 1_555 1_555 1_555 # 32 Check

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

PLAT703_ALERT_1_C Torsion Calc -179.27(15), Rep -179.0(2), Dev.. 1.80 Sigma
C(7)-C(10-C(12-C(13 1_555 1_555 1_555 1_555 # 34 Check

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

PLAT703_ALERT_1_C Torsion Calc 176.17(12), Rep 176.3(2), Dev.. 1.08 Sigma
C(8)-C(11-C(15-S(1) 1_555 1_555 1_555 1_555 # 38 Check

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

PLAT703_ALERT_1_C Torsion Calc 159.71(16), Rep 159.4(2), Dev.. 1.94 Sigma
C(8)-C(11-C(16-N(5) 1_555 1_555 1_555 1_555 # 40 Check

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

```
PLAT703_ALERT_1_C Torsion Calc      -7.2(2), Rep      -6.9(3), Dev..      1.50 Sigma
C(16-C(11-C(15-S(1)  1_555  1_555  1_555  1_555      #      44 Check
```

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

```
PLAT703_ALERT_1_C Torsion Calc  175.07(15), Rep      175.3(2), Dev..      1.53 Sigma
C(16-C(11-C(15-C(7)  1_555  1_555  1_555  1_555      #      45 Check
```

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

```
PLAT703_ALERT_1_C Torsion Calc   -0.35(18), Rep      -0.1(2), Dev..      1.39 Sigma
C(10-C(12-C(18-N(4)  1_555  1_555  1_555  1_555      #      46 Check
```

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

```
PLAT703_ALERT_1_C Torsion Calc  177.72(16), Rep      177.5(2), Dev..      1.38 Sigma
C(10-C(12-C(18-C(14  1_555  1_555  1_555  1_555      #      47 Check
```

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

```
PLAT703_ALERT_1_C Torsion Calc   -3.0(3), Rep      -3.4(5), Dev..      1.33 Sigma
C(13-C(12-C(18-C(14  1_555  1_555  1_555  1_555      #      49 Check
```

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



Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF	Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	1 Report
H3	
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size ..	0.64 mm
PLAT128_ALERT_4_G Alternate Setting for Input Space Group P21/a	P21/c Note
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 !

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

42 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
 1 ALERT type 3 Indicator that the structure quality may be low
 4 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. 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__142611_1
;
PROBLEM: The number of reflections greater than the sigma threshold
RESPONSE: ...
;
_vrf_DIFMN03__142611_1
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
```



```

;
_vrf_DIFMX02__142611_1
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT029__142611_1
;
PROBLEM: _diffn_measured_fraction_theta_full value Low .      0.942 Why?
RESPONSE: ...
;
_vrf_PLAT230__142611_1
;
PROBLEM: Hirshfeld Test Diff for      S1      --O2      .      9.1 s.u.
RESPONSE: ...
;
_vrf_PLAT166__142611_1
;
PROBLEM: S.U's Given on Coordinates for Calc-flagged ....      H1 Note
RESPONSE: ...
;
_vrf_PLAT220__142611_1
;
PROBLEM: NonSolvent      Resd 1  C      Ueq(max)/Ueq(min) Range      3.1 Ratio
RESPONSE: ...
;
# end Validation Reply Form

```

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

