

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

No syntax errors found. CIF dictionary Interpreting this report

Bond precision:	C-C = 0.0041 Å	Wavelength=1.54187	
Cell:	a=6.5525 (5) alpha=94.599 (4)	b=8.5010 (6) beta=98.210 (4)	c=14.9131 (10) gamma=105.947 (4)
Temperature:	293 K		
	Calculated	Reported	
Volume	784.30 (10)	784.30 (10)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C17 H15 N3 O2 S	C17 H15 N3 O2 S	
Sum formula	C17 H15 N3 O2 S	C17 H15 N3 O2 S	
Mr	325.38	325.38	
Dx, g cm-3	1.378	1.378	
Z	2	2	
Mu (mm-1)	1.947	1.947	
F000	340.0	340.0	
F000'	341.61		
h, k, lmax	8, 10, 18	8, 10, 18	
Nref	3068	2727	
Tmin, Tmax	0.775, 0.856	0.711, 0.857	
Tmin'	0.621		

Data completeness= 0.889                      Theta(max)= 71.590

```
R(reflections)= 0.0584( 6289)      wR2(reflections)=
S = 1.106                          0.0816( 6331)
Npar= 259
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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.

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### Alert level A

PLAT029\_ALERT\_3\_A \_diffn\_measured\_fraction\_theta\_full value Low . 0.889 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.**

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### Alert level B

DIFMN02\_ALERT\_2\_B The minimum difference density is < -0.1\*ZMAX\*1.00  
\_refine\_diff\_density\_min given = -1.880  
Test value = -1.600  
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 = 2727  
Number of reflections greater than sigma threshold = 6289  
PLAT097\_ALERT\_2\_B Large Reported Max. (Positive) Residual Density 2.57 eA-3  
PLAT098\_ALERT\_2\_B Large Reported Min. (Negative) Residual Density -1.88 eA-3  
PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for S1 --O3 . 15.7 s.u.  
PLAT703\_ALERT\_1\_B Torsion Calc 173.7(2), Rep 174.2(2), Dev.. 2.50 Sigma  
C(7)-N(5)-N(6)-C(19) 1\_555 1\_555 1\_555 1\_555 # 19 Check

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### 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  
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 .... 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  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C22 Check  
PLAT245\_ALERT\_2\_C U(iso) H2 Smaller than U(eq) C14 by 0.022 Ang\*\*2  
PLAT245\_ALERT\_2\_C U(iso) H11 Smaller than U(eq) C20 by 0.035 Ang\*\*2  
PLAT245\_ALERT\_2\_C U(iso) H12 Smaller than U(eq) C17 by 0.026 Ang\*\*2  
PLAT245\_ALERT\_2\_C U(iso) H14 Smaller than U(eq) C23 by 0.013 Ang\*\*2  
PLAT245\_ALERT\_2\_C U(iso) H15 Smaller than U(eq) C22 by 0.016 Ang\*\*2  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00412 Ang.  
PLAT703\_ALERT\_1\_C Torsion Calc 61.85(19), Rep 61.5(2), Dev.. 1.84 Sigma

	O(2)-S(1)-N(6)-C(19	1_555	1_555	1_555	1_555	#	2	Check
PLAT703_ALERT_1_C	Torsion Calc	177.09(18),	Rep	176.8(2),	Dev..			1.61 Sigma
	C(12)-S(1)-N(6)-C(19	1_555	1_555	1_555	1_555	#	12	Check
PLAT703_ALERT_1_C	Torsion Calc	-179.2(3),	Rep	-179.6(3),	Dev..			1.33 Sigma
	C(16)-C(10)-C(15)-C(14	1_555	1_555	1_555	1_555	#	43	Check

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### ● 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)		0.004 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_reflms_av_unetI/netI .....		Please Do !
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
  - 6 **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
- 
- 12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  - 10 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
  - 12 ALERT type 4 Improvement, methodology, query or suggestion
  - 2 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_DIFMN02__143660_1
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*1.00
RESPONSE: ...
;
_vrf_REFLT02__143660_1
;
PROBLEM: The number of reflections greater than the sigma threshold
RESPONSE: ...
;
_vrf_DIFMN03__143660_1
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_DIFMX02__143660_1
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT097__143660_1
```

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;
PROBLEM: Large Reported Max.   (Positive) Residual Density      2.57 eA-3
RESPONSE: ...
;
_vrf_PLAT098__143660_1
;
PROBLEM: Large Reported Min.   (Negative) Residual Density     -1.88 eA-3
RESPONSE: ...
;
_vrf_PLAT230__143660_1
;
PROBLEM: Hirshfeld Test Diff for    S1          --O3          .      15.7 s.u.
RESPONSE: ...
;
_vrf_PLAT703__143660_1
;
PROBLEM: Torsion Calc    173.7(2), Rep    174.2(2), Dev..      2.50 Sigma
RESPONSE: ...
;
_vrf_PLAT166__143660_1
;
PROBLEM: S.U.'s Given on Coordinates for Calc-flagged ....      H1 Note
RESPONSE: ...
;
_vrf_PLAT241__143660_1
;
PROBLEM: High    'MainMol' Ueq as Compared to Neighbors of      C22 Check
RESPONSE: ...
;
_vrf_PLAT245__143660_1
;
PROBLEM: U(iso) H2          Smaller than U(eq) C14          by      0.022 Ang**2
RESPONSE: ...
;
_vrf_PLAT340__143660_1
;
PROBLEM: Low Bond Precision on   C-C Bonds .....      0.00412 Ang.
RESPONSE: ...
;
# end Validation Reply Form

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

