# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) am105\_lt\_auto

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No syntax errors found. CIF dictionary Interpreting this report

# Datablock: am105\_lt\_auto

Bond precision:	C-C = 0.0022 A	Wavelength=1.54184		
Cell:	a=5.5312(1)	b=13.5140(2)	c=19.5709(3)	
	alpha=90	beta=94.757(1)	gamma=90	
Temperature:	150 K			
	Calculated	Reported		
Volume	1457.86(4)	1457.86(4	1)	
Space group	P 21/c	P 1 21/c	1	
Hall group	-P 2ybc	-P 2ybc		
Moiety formula	C15 H20 N2 O S	C15 H20 N	12 O S	
Sum formula	C15 H20 N2 O S	C15 H20 N	12 O S	
Mr	276.39	276.39		
Dx,g cm-3	1.259	1.255		
Z	4	4		
Mu (mm-1)	1.916	1.915		
F000	592.0	588.0		
F000′	594.77			
h,k,lmax	7,17,24	7,16,24		
Nref	3136	3043		
Tmin,Tmax	0.672,0.713	0.387,1.0	000	
Tmin'	0.610			
Correction metho AbsCorr = MULTI	od= # Reported T I -SCAN	Limits: Tmin=0.387 Tn	nax=1.000	
Data completene	ss= 0.970	Theta(max) = 78.81	0	
R(reflections)=	0.0391( 2754)		wR2(reflections)= 0.0981(3043)	
S = 1.059	Npar=	173		

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

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)	. Please C	Check
PLAT230_ALERT_2_C Hirshfeld Test Diff for S1C2 .	6.0 s	s.u.
PLAT420_ALERT_2_C D-H Bond Without Acceptor N2H2 .	Please C	Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	2.152 0	Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	) 4 F	Report
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.98Ang From N2 .	-0.52 e	eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2 .	-0.38 €	eA-3

## Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	1	Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	76	Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	5	Note
<code>PLAT953_ALERT_1_G</code> Reported (CIF) and Actual (FCF) <code>Hmax Differ</code> by .	1	Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	10	Info

0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
5 ALERT level G = General information/check it is not something unexpected
2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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

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

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## Publication of your CIF in other journals

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PLATON version of 06/07/2023; check.def file version of 30/06/2023

Datablock am105\_lt\_auto - ellipsoid plot



# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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No syntax errors found. CIF dictionary Interpreting this report

## **Datablock: shelx**

Bond precision:	C-C = 0.0019 A	Wavelength=0.71073		
Cell:	a=7.9426(3)	b=23.3394(5)	c=8.9398(3)	
	alpha=90	beta=112.789(4)	gamma=90	
Temperature:	150 K			
	Calculated	Reported		
Volume	1527.85(10)	1527.85(9	)	
Space group	P 21/n	P 21/n		
Hall group	-P 2yn	-P 2yn		
Moiety formula	C16 H22 N2 O S	C16 H22 N	2 O S	
Sum formula	C16 H22 N2 O S	C16 H22 N	2 O S	
Mr	290.42	290.42		
Dx,g cm-3	1.263	1.262		
Z	4	4		
Mu (mm-1)	0.210	0.210		
F000	624.0	624.0		
F000′	624.70			
h,k,lmax	11,33,12	10,33,12		
Nref	4768	4025		
Tmin,Tmax	0.933,0.959	0.460,1.0	00	
Tmin'	0.922			
Correction metho AbsCorr = MULTI	od= # Reported T I -SCAN	Limits: Tmin=0.460 Tm	ax=1.000	
Data completene	ss= 0.844	Theta(max) = 30.75	2	
R(reflections)=	0.0351( 3518)		wR2(reflections)= 0.0909(4025)	
S = 1.054	Npar=	183		

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Click on the hyperlinks for more details of the test.

## ➔ Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for	or Sl	C2		5.2 s.u.
PLAT414_ALERT_2_C Short Intra D-HH-X	H2	H11		1.97 Ang.
		x,y,z	=	1_555 Check
PLAT976_ALERT_2_C Check Calcd Resid. Der	ns. 0.96Ang	From N2	•	-0.41 eA-3

## Alert level G

PLAT007_ALERT_5_G Nu	umber of Unrefined Donor-H Atoms	1	Report
PLAT883_ALERT_1_G No	o Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT899_ALERT_4_G SH	HELXL2018 is Deprecated and Succeeded by SHELXL	2019/3	Note
PLAT910_ALERT_3_G Mi	issing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G Mi	issing # of FCF Reflections Above STh/L= 0.600	698	Note
PLAT978_ALERT_2_G Nu	umber C-C Bonds with Positive Residual Density.	13	Info

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Datablock shelx - ellipsoid plot



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## **Datablock: shelx**

Bond precision:	C-C = 0.0021 A	Wavelength=0.71073		
Cell:	a=6.8186(2)	b=10.0318(2)	c=13.2816(3)	
	alpha=89.529(2)	beta=78.134(2)	gamma=89.102(2)	
Temperature:	150 K			
	Calculated	Reported		
Volume	888.97(4)	888.96(4)		
Space group	P -1	P -1		
Hall group	-P 1	-P 1		
Moiety formula	C20 H15 N3 O3 S	C20 H15 N	13 03 S	
Sum formula	C20 H15 N3 O3 S	C20 H15 N	13 03 S	
Mr	377.41	377.41		
Dx,g cm-3	1.410	1.406		
Z	2	2		
Mu (mm-1)	0.209	0.209		
F000	392.0	390.0		
F000′	392.41			
h,k,lmax	9,14,19	8,13,17		
Nref	5649	4318		
Tmin,Tmax	0.951,0.962	0.664,1.0	000	
Tmin'	0.951			
Correction metho	od= # Reported T Li	mits: Tmin=0.664 Tm	nax=1.000	
AbsCorr = MULTI-	-SCAN			
Data completenes	ss= 0.764	Theta(max) = 30.94	1	
R(reflections)=	0.0389( 3503)		wR2(reflections) =	
S = 1.072	Npar= 2	44	U.IUUZ( 4318)	

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## Alert level C

PLAT068_ALERT_1_C	Reported F0	00 Differs fr	om Calcd	(or Missin	g)	Please Check
PLAT911_ALERT_3_C	Missing FCF	Refl Between	Thmin &	STh/L=	0.600	40 Report

## Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	1 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal (Note)	0.002 Degree
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).	2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	1037 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	2.5 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.	2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.	2 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	11 Info

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