

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait ..

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) feba391

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.

Please wait while processing

[CIF dictionary](#)

[Interpreting this report](#)

[Structure factor report](#)

Datablock: feba391

Bond precision:	C-C = 0.0054 Å	Wavelength=0.71073
Cell:	a=11.544(3) b=13.204(3) c=10.086(3)	
	alpha=90 beta=112.081(7) gamma=90	
Temperature:	130 K	

	Calculated	Reported
Volume	1424.6(7)	1424.6(6)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C12 H17 N5 O S	C12 H17 N5 O S
Sum formula	C12 H17 N5 O S	C12 H17 N5 O S
Mr	279.37	279.36
Dx, g cm ⁻³	1.303	1.303
Z	4	4
Mu (mm ⁻¹)	0.228	0.228
F000	592.0	592.0
F000'	592.67	
h,k,lmax	13,15,12	13,15,12
Nref	2634	2577
Tmin,Tmax	0.955,0.998	0.956,0.998
Tmin'	0.955	

Correction method= # Reported T Limits: Tmin=0.956
Tmax=0.998 AbsCorr = MULTI-SCAN

Data completeness= 0.978 Theta(max)= 25.452

R(reflections)= 0.0577(1664) wR2(reflections)= 0.1609(2577)

S = 1.025 Npar= 172

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

PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00537 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H4A ..S1	2.94 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H11A ..S1	2.97 Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1 Note
	C12 H17 N5 O S	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.778 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	26 Report

Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	3	Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1	109.2	Degree
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	30	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	7	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 6 **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
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 3 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 ALERT type 3 Indicator that the structure quality may be low
 4 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

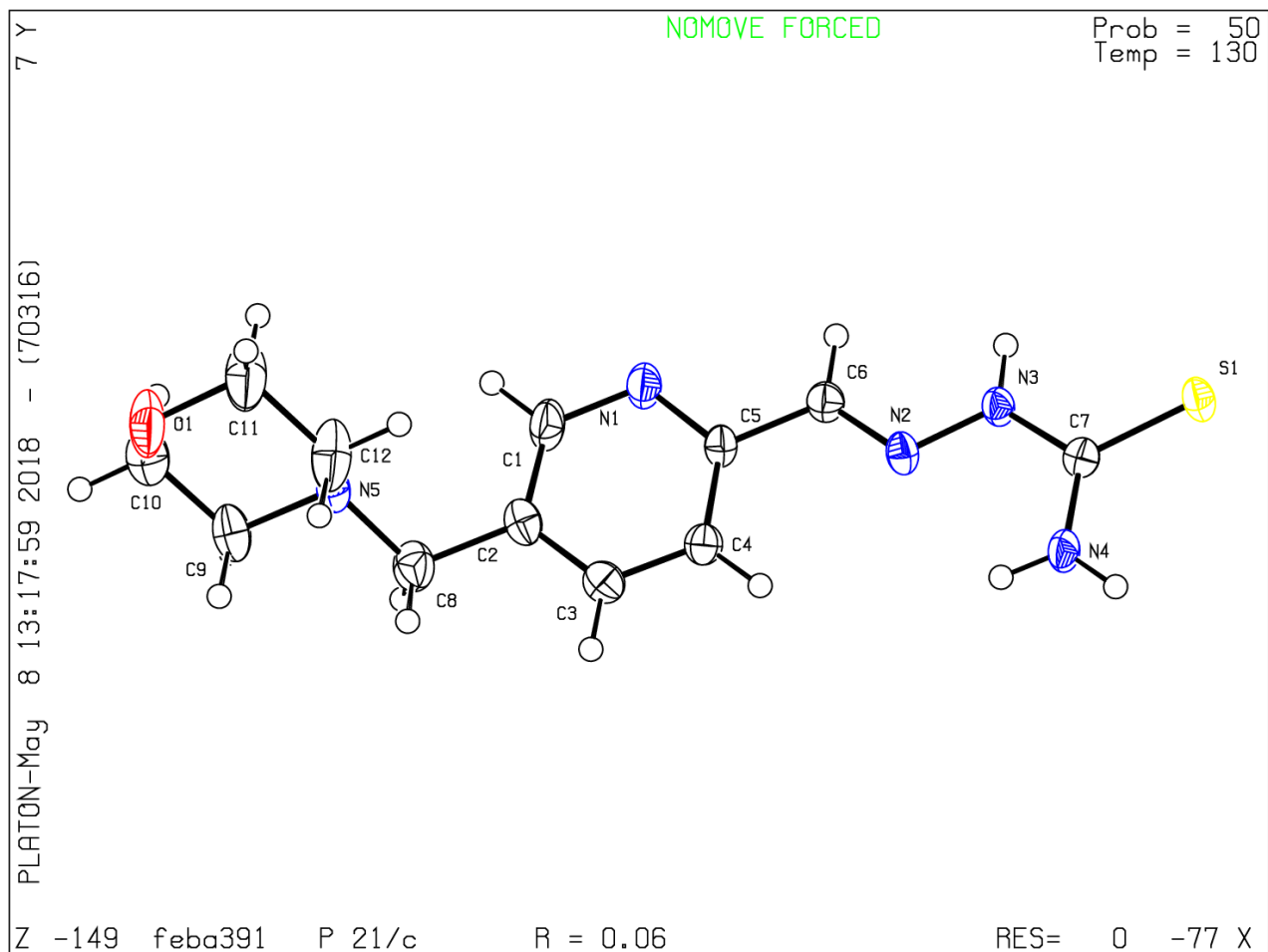
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

PLATON version of 23/04/2018; check.def file version of 23/04/2018

Datablock feba391 - ellipsoid plot



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