No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Datablock: b

Bond precision: C-C = 0.0032 A Wavelength=0.71073
Cell: a=9.7377(19) b=11.142(2) c=11.584(2)
alpha=71.62(3) beta=67.21(3) gamma=86.01(3)
Temperature : 293 K

	Calculated	Reported
Volume	1097.6(5)	1097.6(4)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C10 H10 N4 O2 S, 2(C5 H9 N O)	?
Sum formula	C20 H28 N6 O4 S	C20 H28 N6 O4 S
Mr	448.54	448.54
Dx,g cm-3	1.357	1.357
Z	2	2
Mu (mm-1)	0.187	0.187
F000	476.0	476.0
F000'	476.43	
h,k,lmax	12,14,15	12,14,15
Nref	5292	5197
Tmin,Tmax	0.967,0.981	0.964,0.982
Tmin'	0.963	

Correction method= # Reported T Limits: Tmin=0.964
Tmax=0.982 AbsCorr = ?
Data completeness= 0.982 Theta(max)= 27.970
R(reflections)= 0.0412(2846) wR2(reflections)= 0.1140(5197)
S = 1.005 Npar= 281

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

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	N5	Check

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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	3	Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed	Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.03	Degree
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) O3 -- C11 ..	5.7	s.u.
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C20	Check
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014	Note

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
4 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

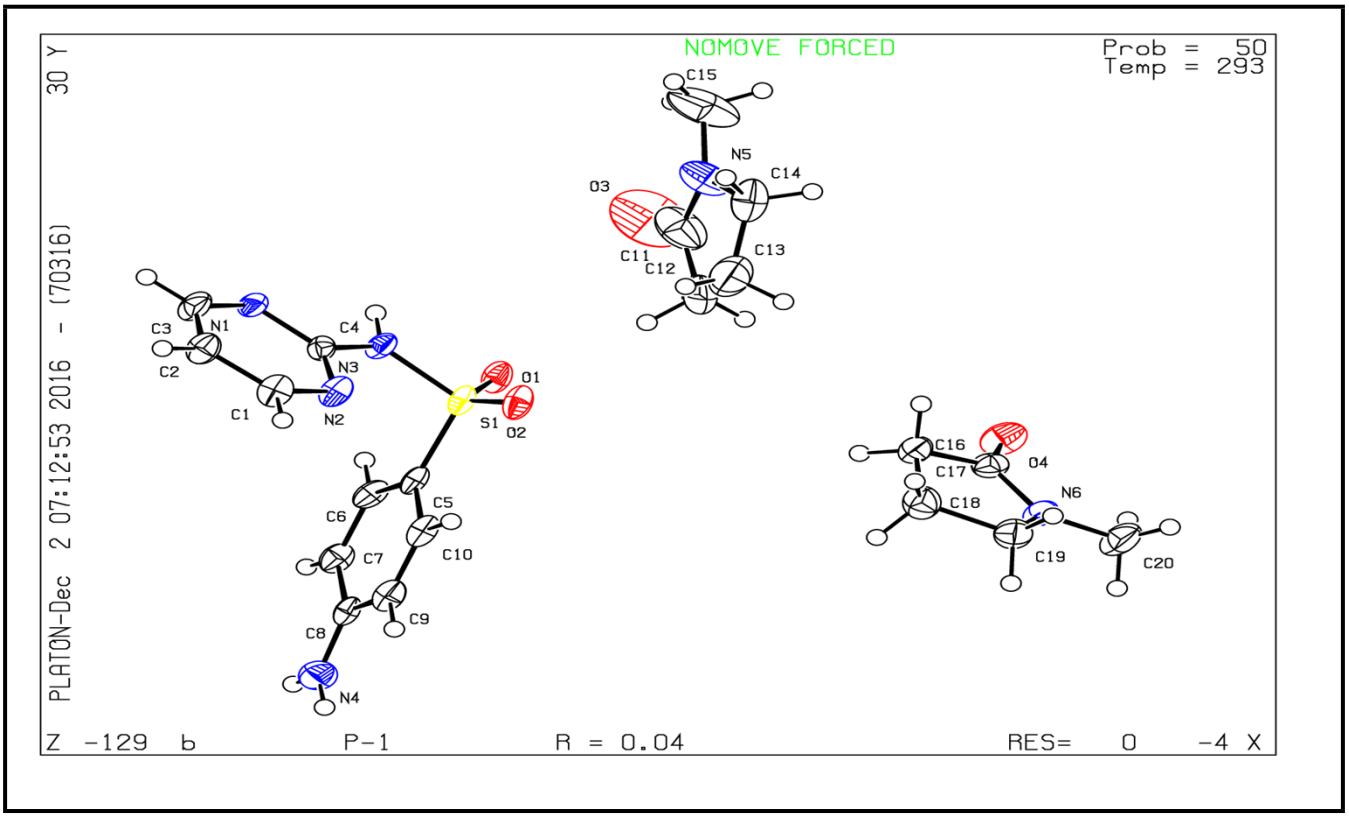
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

PLATON version of 24/11/2016; check.def file version of 23/11/2016

Datablock b - ellipsoid plot



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