

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Dmap-H_Tos

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: Dmap-H_Tos

Bond precision: C-C = 0.0020 Å Wavelength=1.54184

Cell: a=7.0280 (3) b=8.1296 (4) c=13.1100 (6)
 alpha=72.873 (4) beta=79.560 (4) gamma=80.826 (4)
Temperature: 120 K

	Calculated	Reported
Volume	699.47 (6)	699.47 (6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C7 H7 O3 S, C7 H11 N2	C7 H7 O3 S, C7 H11 N2
Sum formula	C14 H18 N2 O3 S	C14 H18 N2 O3 S
Mr	294.36	294.36
Dx, g cm ⁻³	1.398	1.398
Z	2	2
Mu (mm ⁻¹)	2.144	2.144
F000	312.0	312.0
F000'	313.55	
h, k, lmax	8, 9, 15	8, 9, 15
Nref	2481	2477
Tmin, Tmax	0.773, 0.876	0.843, 1.000
Tmin'	0.773	

Correction method= # Reported T Limits: Tmin=0.843 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.998 Theta(max)= 66.734

R(reflections)= 0.0301 (2402)	wR2(reflections)=
S = 1.072	0.0801 (2477)
Npar= 184	

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

PLAT353_ALERT_3_C	Long N-H (N0.87,N1.01A) N1 - H1 .	1.04 Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.596	5 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)	0.004 Degree
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3 Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	96% Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.0 Low
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	133.5 Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	13 Info

- 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
8 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
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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.

