

No syntax errors found.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

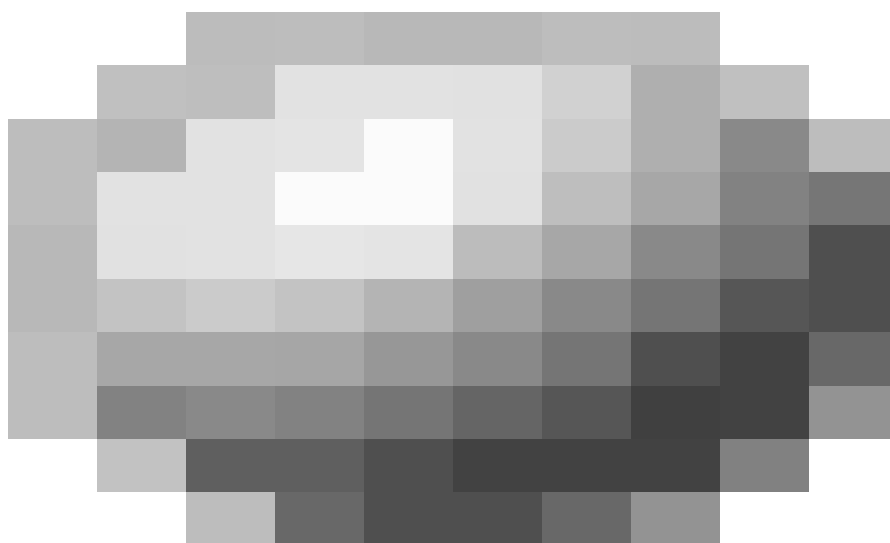
Datablock: 1x2H2O

Bond precision: C-C = 0.0032 Å Wavelength=0.71073
Cell: a=7.2258(14) b=8.0470(16) c=11.287(2)
alpha=70.71(3) beta=74.88(3) gamma=79.85(3)

Temperature 293 K
:

	Calculated	Reported
Volume	595.1(2)	595.1(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C11 H10 N2 O2, 2(H2 O)	C11 H14 N2 O4
Sum formula	C11 H14 N2 O4	C11 H14 N2 O4
Mr	238.24	238.24
Dx, g cm-3	1.330	1.330
Z	2	2
Mu (mm-1)	0.102	0.102
F000	252.0	252.0
F000'	252.14	
h, k, lmax	8, 9, 13	8, 9, 13
Nref	2182	2183
Tmin, Tmax	0.955, 0.984	0.518, 1.000
Tmin'	0.916	
Correction method=	# Reported T Limits: Tmin=0.518	
Tmax=1.000 AbsCorr =	GAUSSIAN	
Data completeness=	1.000 Theta(max)= 25.341	
R(reflections)=	0.0492(1649) wR2(reflections)= 0.1446(2183)	
S =	1.033 Npar= 166	

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 G

[PLAT002_ALERT_2_G](#) Number of Distance or Angle Restraints on AtSite
[PLAT005_ALERT_5_G](#) No Embedded Refinement Details Found in the CIF
[PLAT007_ALERT_5_G](#) Number of Unrefined Donor-H Atoms

6 Note
Please Do !
1 Report

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT063_ALERT_4_G	Crystal Size Possibly too Large for Beam Size ..	0.86 mm
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 _diffn_ambient_temperature (K)	293 Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp ²)-Methyl Moiety	C11 Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	2 Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	3 Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	4 Note

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

- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 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 05/12/2020; check.def file version of 05/12/2020

Datablock 1x2H2O - ellipsoid plot

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