checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: C-C = 0.0015 A Wavelength=0.71073

Cell: a=4.9756(2) b=11.5590(5) c=14.9966(7)
alpha=76.210(2) beta=80.870(2) gamma=78.172(1)
Temperature: 100 K

	Calculated	Reported
Volume	814.36(6)	814.36(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	Cl0.10 H2 O, 2(C4 H10 N3 O2), 1.898(Cl)	2(C4 H10 N3 O2), 2Cl, H2 O
Sum formula	C8 H22 Cl2 N6 O5	C8 H22 Cl2 N6 O5
Mr	353.22	353.21
Dx,g cm-3	1.441	1.440
Z	2	2
Mu (mm-1)	0.428	0.428
F000	372.0	372.0
F000’	372.74	
h,k,lmax	7,16,21	7,16,21
Nref	5000	4985
Tmin,Tmax	0.893,0.958	0.904,1.000
Tmin’	0.868	

Correction method= # Reported T Limits: Tmin=0.904 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 30.558

R(reflections)= 0.0259(4498) wR2(reflections)= 0.0711(4985)

S = 1.033 Npar= 239

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 B

PLAT780_ALERT_1_B Coordinates do not Form a Properly Connected Set Please Do !

Alert level C

PLAT303_ALERT_2_C Full Occupancy Atom H1O with # Connections 1.05 Check
PLAT303_ALERT_2_C Full Occupancy Atom H2O with # Connections 1.05 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 8 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 4 Note

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 19 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 4 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 3 Note
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 9% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 10 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 14 Note
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 6 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
5 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 05/12/2020; check.def file version of 05/12/2020

Datablock shelx - ellipsoid plot