checkCIF/PLATON report

Structure factors have been supplied for datablock(s) gellman186_sq

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: gellman186_sq

Bond precision: C-C = 0.0073 A Wavelength=0.71073

Cell: a=17.997(6) b=6.1519(18) c=19.636(6)
alpha=90 beta=106.549(11) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2084.0(11)	2083.9(11)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C21 H20 N O2, Cl [+ solvent]	Cl, C21 H20 N O2
Sum formula	C21 H20 Cl N O2 [+ solvent]	C21 H20 Cl N O2
Mr	353.83	353.83
Dx,g cm-3	1.128	1.128
Z	4	4
Mu (mm-1)	0.195	0.195
F000	744.0	744.0
F000’	744.88	
h,k,lmax	22,7,24	22,7,24
Nref	4308	4282
Tmin,Tmax	0.981,0.985	0.524,0.745
Tmin’	0.981	

Correction method= # Reported T Limits: Tmin=0.524 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 26.441

R(reflections)= 0.0972(3810) wR2(reflections)= 0.2745(4282)

S = 1.057 Npar= 229

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

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 1.89 eA-3

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

Author Response: The maximum peak (ca. 1.87 electons/\%A^3^) is 0.90 \%A from atom Cl1 in a chemically unreasonable position and was considered noise.

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.27 Report

Author Response: Due to the lower than usual data quality resulting from the challenging (twinned) nature of the crystal and the need to process the data with SQUEEZE, this was the best attainable wR2 value for a chemically reasonable model of the structure.

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.16 Report

Author Response: The large ratio is due to a feature in the difference Fourier map: the maximum peak (ca. 1.87 electrons/\%A^3^) is 0.90 \%A from atom Cl1 in a chemically unreasonable position that was considered noise.

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00732 Ang.

Author Response: Due to the lower than usual data quality resulting from the challenging (twinned) nature of the crystal and the need to process the data with SQUEEZE, this was the best attainable precision for a chemically reasonable model of the structure.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.443 Check

Author Response: Usually data integration algorithms underestimate the background and produces slightly elevated values of Fo, resulting in higher Fo/Fc values. These are most pronounced for the weakest intensities.

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 3 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.17 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 194 A**3
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 16 Note

PLAT931_ALERT_5_G CIFcalcFCF Twin Law (1 0 0) Est.d BASF 0.24 Check

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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
5 **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

2 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
3 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 03/05/2019; check.def file version of 29/04/2019

Datablock gellman186_sq - ellipsoid plot