checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 7_sq_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: 7_sq_sq

Bond precision: C-C = 0.0109 A Wavelength=1.54184

Cell: a=14.6457(2) b=16.7294(4) c=22.7944(5)
alpha=88.152(2) beta=76.205(2) gamma=67.284(2)
Temperature: 100 K

	Calculated	Reported
Volume	4992.0(2)	4991.95(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C104 H78, 2(C2 H4 Cl2) [+ solvent]	C2 H4 Cl2, 0.5(C104 H78)
Sum formula	C108 H86 Cl4 [+ solvent]	C54 H43 Cl2
Mr	1525.57	762.78
Dx,g cm-3	1.015	1.015
Z	2	4
Mu (mm-1)	1.391	1.391
F000	1604.0	1604.0
F000'	1610.66	
h,k,lmax	17,20,27	17,20,26
Nref	18027	17355
Tmin,Tmax	0.905,0.959	0.965,0.985
Tmin'	0.870	

Correction method= # Reported T Limits: Tmin=0.965 Tmax=0.985
AbsCorr = MULTI-SCAN

Data completeness= 0.963 Theta(max)= 67.584

R(reflections)= 0.1500(14829) wR2(reflections)= 0.3395(17355)

S = 1.039 Npar= 1021

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

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01089 Ang.

Alert level C

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

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full value Low .	0.963 Why?
PLAT082_ALERT_2_C	High R1 Value	0.15 Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.34 Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	1.52 eA-3
PLAT213_ALERT_2_C	Atom C03C has ADP max/min Ratio	4.0 prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	4.1 Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.6 Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C02Z --C031 .	0.17 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C039 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C033 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	14.319 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.145 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.068 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	649 Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	3 Check
PLAT977_ALERT_2_C	Check Negative Difference Density on H02D	-0.33 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H0AA	-0.37 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H030	-0.31 eA-3

Alert level G

PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ	Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50 Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	66.34 Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002 Degree
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	! Info
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	195 Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	! Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	66% Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.3 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
19 **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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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 12 ALERT type 2 Indicator that the structure model may be wrong or deficient
 11 ALERT type 3 Indicator that the structure quality may be low
  4 ALERT type 4 Improvement, methodology, query or suggestion
  0 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.

PLATON version of 13/07/2021; check.def file version of 13/07/2021

Datablock 7_sq_sq - ellipsoid plot