

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 6cl

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: 6cl

Bond precision: C-C = 0.0064 A Wavelength=1.54178

Cell: a=7.4787(6) b=12.4743(8) c=21.0321(14)
 alpha=83.940(6) beta=82.931(6) gamma=82.882(6)

Temperature: 113 K

	Calculated	Reported
Volume	1924.1(2)	1924.1(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C42 H38 Cl6 N2 O6	2(C21 H19 Cl3 N O3)
Sum formula	C42 H38 Cl6 N2 O6	C42 H38 Cl6 N2 O6
Mr	879.44	879.44
Dx,g cm-3	1.518	1.518
Z	2	2
Mu (mm-1)	4.512	4.512
F000	908.0	908.0
F000'	914.56	
h,k,lmax	8,14,24	8,14,23
Nref	6157	5943
Tmin,Tmax	0.759,0.914	0.903,1.000
Tmin'	0.100	

Correction method= # Reported T Limits: Tmin=0.903 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.965 Theta(max)= 62.562

R(reflections)= 0.0793(4376) wR2(reflections)= 0.2132(5943)

S = 1.081 Npar= 483

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

PLAT936_ALERT_2_B The Embedded .res File Includes a DAMP Command . 500.0 Report

Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5756
PLAT018_ALERT_1_C _diffn_measured_fraction_theta_max .NE. *_full ! Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00639 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 7.004 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.107 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.576 206 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers 1 Check

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 32 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 58 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.45 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.006 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 6 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for N1 --C14 6.7 s.u.
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 29% Note
PLAT301_ALERT_3_G Main Residue Disorder(Resd 2) 29% Note
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O3 108.2 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O5 108.8 Degree
PLAT793_ALERT_4_G Model has Chirality at C15 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at C36 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at C15' (Centro SPGR) R Verify
PLAT793_ALERT_4_G Model has Chirality at C36' (Centro SPGR) R Verify
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 136 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 60% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
7 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 23/04/2018; check.def file version of 23/04/2018

