

Datablock: s2

Bond precision:	C-C = 0.0104 A	Wavelength=1.54178
Cell:	a=7.2988(4) b=6.0350(3) c=31.3274(16)	
	alpha=90 beta=90 gamma=90	
Temperature	100 K	
:		
	Calculated	Reported
Volume	1379.92(12)	1379.92(12)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C17 H15 Cl O	C17 H15 Cl O
Sum formula	C17 H15 Cl O	C17 H15 Cl O
Mr	270.74	270.74
Dx,g cm-3	1.303	1.303
Z	4	4
Mu (mm-1)	2.343	2.343
F000	568.0	568.0
F000'	570.84	
h,k,lmax	9,7,39	9,6,37
Nref	1401	1339
Tmin,Tmax	0.755,0.889	0.639,0.754
Tmin'	0.420	
Correction method=	# Reported T Limits: Tmin=0.639	
Tmax=0.754 AbsCorr =	MULTI-SCAN	
Data completeness=	0.956	Theta(max)= 74.222
R(reflections)=	0.1470(1030)	wR2(reflections)= 0.3393(1339)
S = 1.151	Npar= 101	

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 0.01044 Ang.



Alert level C

[PLAT029_ALERT_3_C](#) diffrn_measured_fraction_theta_full value Low . 0.973 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
[PLAT336_ALERT_2_C](#) Long Bond Distance for Cl -Cl1 1.876 Ang.
[PLAT906_ALERT_3_C](#) Large K Value in the Analysis of Variance 32.708 Check

And 2 other PLAT906 Alerts

[PLAT906_ALERT_3_C](#) Large K Value in the Analysis of Variance 7.335 Check
[PLAT906_ALERT_3_C](#) Large K Value in the Analysis of Variance 3.222 Check

[PLAT911_ALERT_3_C](#) Missing FCF Refl Between Thmin & STh/L= 0.600 21 Report



Alert level G

[PLAT002_ALERT_2_G](#) Number of Distance or Angle Restraints on AtSite 2 Note
[PLAT083_ALERT_2_G](#) SHELXL Second Parameter in WGHT Unusually Large 11.10 Why ?
[PLAT172_ALERT_4_G](#) The CIF-Embedded .res File Contains DFIX Records 1 Report
[PLAT300_ALERT_4_G](#) Atom Site Occupancy of Cl1 Constrained at 0.5 Check

And 5 other PLAT300 Alerts

[PLAT300_ALERT_4_G](#) Atom Site Occupancy of O1 Constrained at 0.5 Check
[PLAT300_ALERT_4_G](#) Atom Site Occupancy of C9 Constrained at 0.5 Check
[PLAT300_ALERT_4_G](#) Atom Site Occupancy of H9A Constrained at 0.5 Check
[PLAT300_ALERT_4_G](#) Atom Site Occupancy of H9B Constrained at 0.5 Check

PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	16%	Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1		104.3	Degree
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		6	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	6	Note
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ		2	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ		2	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		1	Info

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 6 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
 9 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

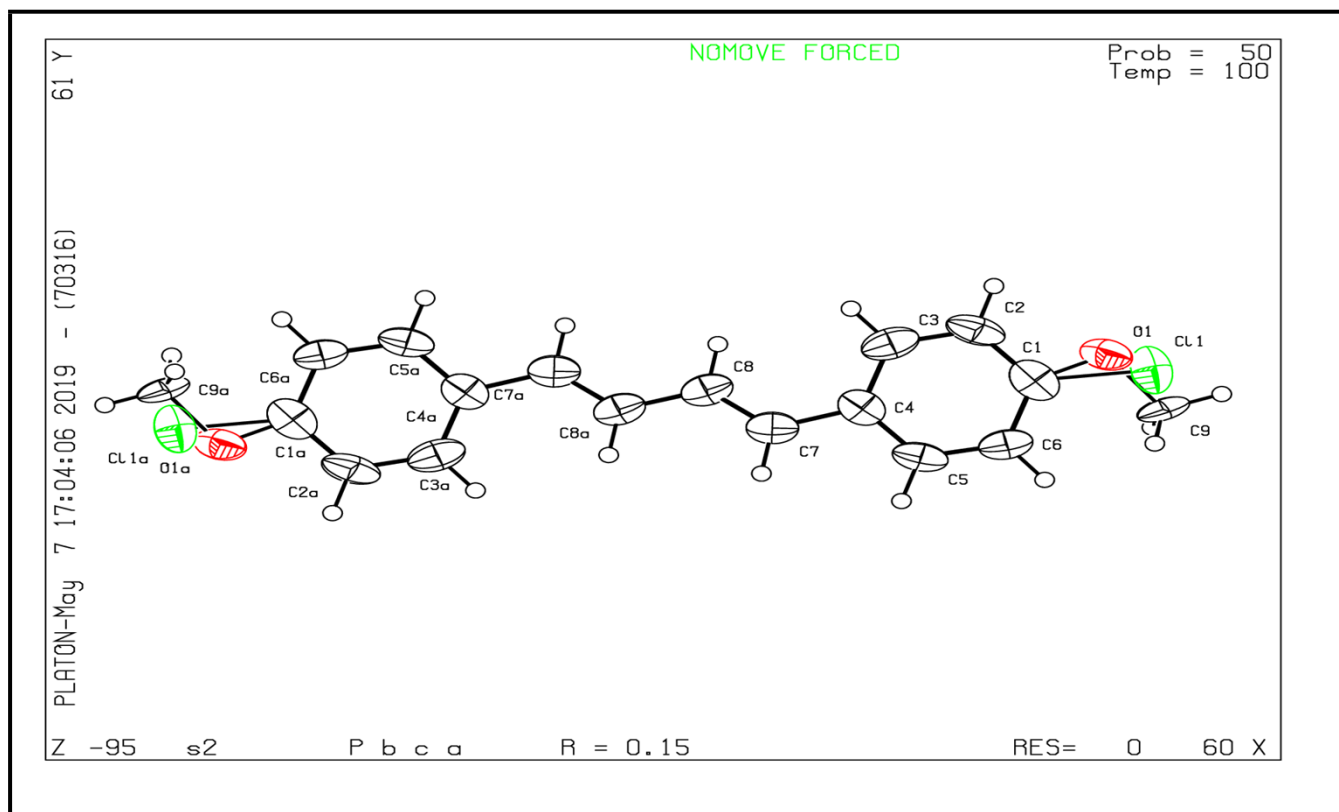
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 03/05/2019; check.def file version of 29/04/2019

Datablock s2 - ellipsoid plot



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