

checkCIF (basic structural check) running

checkCIF/PLATON (basic structural check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

Datablock: p-1

Bond precision:	C-C = 0.0126 A	Wavelength=0.71073
Cell:	a=10.647(2) b=11.562(2) c=11.666(2)	
	alpha=79.59(3) beta=84.08(3) gamma=68.05(3)	
Temperature:	293 K	
	Calculated	Reported
Volume	1309.1(5)	1309.1(4)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	C26 H29 Cl Ir N3 O2, C H4 O	?
Sum formula	C27 H33 Cl Ir N3 O3	C27 H33 Cl Ir N3 O3
Mr	675.23	675.21
Dx, g cm ⁻³	1.713	1.713
Z	2	2
Mu (mm ⁻¹)	5.235	5.235
F000	668.0	668.0
F000'	665.71	
h,k,lmax	12,13,13	12,13,13
Nref	4562	4542
Tmin,Tmax	0.471,0.552	0.655,0.915
Tmin'	0.455	
Correction method=	# Reported T Limits: Tmin=0.655 Tmax=0.915 AbsCorr =	
	NUMERICAL	
Data completeness=	0.996 Theta(max)= 24.890	
R(reflections)=	0.0481(4119) wR2(reflections)= 0.1278(4542)	
S =	1.107 Npar= 308	

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 C

[PLAT094_ALERT_2_C](#) Ratio of Maximum / Minimum Residual Density 2.59 Report
[PLAT165_ALERT_3_C](#) Nr. of Status R Flagged Non-Hydrogen Atoms 4 Note
[PLAT342_ALERT_3_C](#) Low Bond Precision on C-C Bonds 0.01264 Ang.
[PLAT362_ALERT_2_C](#) Short C(sp3)-C(sp2) Bond C17 - C19 .. 1.38 Ang.
[PLAT362_ALERT_2_C](#) Short C(sp3)-C(sp2) Bond C19 - C20 .. 1.41 Ang.

● Alert level G

[PLAT005_ALERT_5_G](#) No Embedded Refinement Details found in the CIF Please Do !
[PLAT007_ALERT_5_G](#) Number of Unrefined Donor-H Atoms 1 Report
[PLAT154_ALERT_1_G](#) The s.u.'s on the Cell Angles are Equal ..(Note) 0.03 Degree
[PLAT199_ALERT_1_G](#) Reported _cell_measurement_temperature (K) 293 Check
[PLAT200_ALERT_1_G](#) Reported _diffn_ambient_temperature (K) 293 Check
[PLAT720_ALERT_4_G](#) Number of Unusual/Non-Standard Labels 3 Note
[PLAT790_ALERT_4_G](#) Centre of Gravity not Within Unit Cell: Resd. # 2 Note
 C H4 O
[PLAT899_ALERT_4_G](#) SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 0 **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
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- 3 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
 - 2 ALERT type 3 Indicator that the structure quality may be low
 - 3 ALERT type 4 Improvement, methodology, query or suggestion
 - 2 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 30/03/2016; check.def file version of 30/03/2016

Datablock p-1 - ellipsoid plot

