

# checkCIF/PLATON report

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

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: shelx

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Bond precision:    C-C = 0.0071 A

Wavelength=0.71073

Cell:                a=9.1111(3)                b=11.1583(5)                c=17.8104(8)  
                      alpha=77.661(4)            beta=76.942(4)            gamma=81.311(3)  
Temperature:        293 K

	Calculated	Reported
Volume	1713.04(13)	1713.04(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C25 H20 Cl Co N4 O, C6 F4 I2, C H4 O, Cl	C25 H20 Cl Co N4 O, C6 F4 I2, C H4 O, Cl
Sum formula	C32 H24 Cl2 Co F4 I2 N4 O2	C32 H24 Cl2 Co F4 I2 N4 O2
Mr	956.18	956.18
Dx, g cm-3	1.854	1.854
Z	2	2
Mu (mm-1)	2.517	2.517
F000	926.0	926.0
F000'	925.77	
h,k,lmax	10,13,21	10,13,21
Nref	6035	5872
Tmin,Tmax	0.241,0.458	0.624,1.000
Tmin'	0.203	

Correction method= # Reported T Limits: Tmin=0.624 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.973

Theta(max)= 24.999

R(reflections)= 0.0297( 4242)

wR2(reflections)= 0.0655( 5872)

S = 0.940

Npar= 430

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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.

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**Alert level C**

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full	value Low	0.973	Why?
PLAT193_ALERT_1_C	Cell and Diffraction Temperatures Differ by	...	2	Degree
PLAT220_ALERT_2_C	Non-Solvent Resd 1	C Ueq(max)/Ueq(min) Range	4.1	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	I1 --C25 ..	5.5	s.u.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		01	Check
PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist	C25 -C30	1.37	Ang.

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**Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		2	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	.....	1	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		1	Report
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	.... (K)	293	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I1	..Cl1	3.16	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I2	..Cl1	3.16	Ang.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	C6 F4 I2			
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	.....	1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File	...	1	Note

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

2 **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  
2 **ALERT type 3** Indicator that the structure quality may be low  
2 **ALERT type 4** Improvement, methodology, query or suggestion  
1 **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.

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**PLATON version of 09/11/2017; check.def file version of 08/11/2017**

