

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) c134s

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: c134s

Bond precision:	C-C = 0.0160 A	Wavelength=0.71073
Cell:	a=12.709(3)	b=17.045(3) c=24.688(5)
	alpha=90	beta=101.84(3) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	5234(2)	5234.6(19)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C25 H18 Au F5 N O P S), C Cl2.50, 0.5(Cl)	?
Sum formula	C51 H36 Au2 Cl3 F10 N2 O2 P2 S2	C25.50 H18 Au Cl1.50 F5 N O P S
Mr	1525.17	762.58
Dx, g cm-3	1.936	1.935
Z	4	8
Mu (mm-1)	5.972	5.972
F000	2932.0	2932.0
F000'	2921.35	
h,k,lmax	15,20,29	15,20,29
Nref	9745	9695
Tmin,Tmax	0.493,0.620	0.507,1.000
Tmin'	0.122	

Correction method= # Reported T Limits: Tmin=0.507 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 25.498

R(reflections)= 0.0690(8537) wR2(reflections)= 0.1220(9695)

S = 1.315 Npar= 663

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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).

32 Note

Alert level C

PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	2	Check
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	4.0	Ratio
PLAT220_ALERT_2_C	Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range	4.7	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 2 H Uiso(max)/Uiso(min) Range	4.5	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C71 --C72 .	0.18	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C31	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C32	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C30	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C71	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C100	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01602	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	12.824	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.605	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	18	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.51A From Cl6	2.21	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.84A From Cl4	2.02	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.83A From Cl5	1.85	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.87A From Cl6	1.80	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.53A From C71	1.70	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.91A From Aul	1.59	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.65A From Cl4	-1.94	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 1.79A From C30	-1.64	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.68A From Cl4	-1.62	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 1.17A From C71	-1.59	eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	1	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
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	83.53	Why ?
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	3	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl2 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl3 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl4 Constrained at	0.7	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl6 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl1 Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl5 Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	71%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 3	3.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 4	0.50	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Cl5 ..C100	2.11	Ang.
	x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Cl1 ..C100	2.82	Ang.
	2-x,1-y,1-z =	3_766	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3 ..F8	2.71	Ang.
	1-x,-y,1-z =	3_656	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	112	Check

CL6	-C100	-CL2	1.555	1.555	1.555	43.10 Deg.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints					9 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...					12 Note
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
24 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
24 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
15 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.

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