

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a

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: a

Bond precision:	C-C = 0.0342 A	Wavelength=1.54184	
Cell:	a=24.0503 (6)	b=12.2870 (2)	c=30.3447 (8)
	alpha=90	beta=109.212 (3)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	8467.7 (4)	8467.7 (4)	
Space group	C 2	C 2	
Hall group	C 2y	C 2y	
Moiety formula	3(C28 H23 Au Cl N3 O), H2 O [+ solvent]	3(C28 H23 Au Cl N3 O), H2 O [+ solvent]	
Sum formula	C84 H71 Au3 Cl3 N9 O4 [+ solvent]	C84 H71 Au3 Cl3 N9 O4	
Mr	1967.76	1967.74	
Dx, g cm-3	1.543	1.544	
Z	4	4	
Mu (mm-1)	10.855	10.855	
F000	3832.0	3832.0	
F000'	3791.65		
h, k, lmax	30, 15, 38	29, 15, 37	
Nref	17643 [9251]	12598	
Tmin, Tmax	0.220, 0.219	0.660, 1.000	
Tmin'	0.141		

Correction method= # Reported T Limits: Tmin=0.660 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.36/0.71 Theta(max)= 75.938

R(reflections)= 0.0562(9952)

wR2(reflections)=
0.1703(12598)

S = 0.900

Npar= 919

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

PLAT201_ALERT_2_B	Isotropic non-H Atoms in Main Residue(s)	2	Report
	C34 C83		
PLAT213_ALERT_2_B	Atom C82 has ADP max/min Ratio	4.4	oblate
PLAT220_ALERT_2_B	NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range	9.6	Ratio
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of	C83	Check
PLAT242_ALERT_2_B	Low 'MainMol' Ueq as Compared to Neighbors of	C78	Check
PLAT242_ALERT_2_B	Low 'MainMol' Ueq as Compared to Neighbors of	C80	Check
PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.0342	Ang.
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O39 --H39A .		Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O39 --H39B .		Please Check
PLAT915_ALERT_3_B	No Flack x Check Done: Low Friedel Pair Coverage	47	%
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 1.18Ang From Au3	2.52	eA-3



Alert level C

PLAT213_ALERT_2_C	Atom C81 has ADP max/min Ratio	3.9	prolat
PLAT222_ALERT_3_C	NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range	8.4	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C18 --C19 .	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C21 --C26 .	0.20	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C31 --C32 .	0.22	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C82	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C41	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C76	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C88	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C77	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N7	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C70	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2)	2.8	Note
PLAT331_ALERT_2_C	Small Aver Phenyl C-C Dist C70 --C75 .	1.37	Ang.
PLAT332_ALERT_2_C	Large Phenyl C-C Range C70 -C75 .	0.18	Ang.
PLAT363_ALERT_2_C	Long C(sp3)-C(sp2) Bond C73 - C78 .	1.63	Ang.
PLAT411_ALERT_2_C	Short Inter H...H Contact H35 ..H77 .	2.14	Ang.
	1/2-x,1/2+y,-z =	4_555	Check
PLAT752_ALERT_4_C	Angle Calc 103.00, Rep 103(6)		Senseless s.u.
	H39A -O39 -H39B 1_555 1_555 1_555 # 60		Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	110	Report
	11 13 0, 22 0 0, -13 13 1, 11 13 1, 21 9 1, 22 0 1,		
	-16 0 2, 11 13 2, 21 9 2, -16 0 3, 11 13 3, -16 0 4,		
	-8 14 4, 2 0 4, 11 13 4, 14 12 4, 18 10 4, 19 9 4,		
	-23 5 5, -16 0 5, -14 10 5, -2 0 5, 14 12 5, 19 9 5,		
	-23 5 6, -16 0 6, -14 10 6, 15 11 6, 20 0 6, -28 0 7,		
	-23 5 7, -16 0 7, -14 10 7, 19 9 7, 20 0 7, -28 0 8,		
	-23 5 8, -16 0 8, -14 10 8, 15 11 8, -28 0 9, -23 5 9,		
	-16 0 9, -14 0 9, -14 10 9, -23 5 10, -16 0 10, -14 0 10,		
	-23 5 11, -16 0 11, 20 6 11, 21 5 11, -24 8 12, -23 5 12,		

-16	0 12,	-14 10 12,	0 8 12,	19 7 12,	20 4 12,	-14 10 13,
0	8 13,	19 3 13,	-23 7 14,	-13 11 14,	18 4 14,	-28 0 15,
-23	5 15,	-23 7 15,	-13 11 15,	-28 0 16,	-22 8 16,	-13 11 16,
-28	0 17,	-13 11 17,	-4 10 17,	-28 0 18,	-16 10 18,	-15 9 18,
-13	11 18,	-4 10 18,	-28 0 19,	-16 10 19,	-13 11 19,	-4 0 19,
-16	10 20,	-13 11 20,	-18 0 21,	-16 10 21,	-13 11 21,	-18 0 22,
-16	10 22,	-18 0 23,	-16 10 23,	1 5 23,	10 0 23,	-18 0 24,
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens.	1.03Ang	From Au1		2.15 eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens.	0.97Ang	From Au2		2.01 eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens.	1.01Ang	From Au1		1.97 eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens.	0.90Ang	From Au2		1.72 eA-3
PLAT972_ALERT_2_C	Check	Calcd Resid. Dens.	0.74Ang	From Au1		-2.25 eA-3
PLAT972_ALERT_2_C	Check	Calcd Resid. Dens.	0.85Ang	From Au1		-2.06 eA-3
PLAT972_ALERT_2_C	Check	Calcd Resid. Dens.	0.74Ang	From Au2		-2.03 eA-3
PLAT972_ALERT_2_C	Check	Calcd Resid. Dens.	0.81Ang	From Au1		-2.02 eA-3
PLAT972_ALERT_2_C	Check	Calcd Resid. Dens.	0.82Ang	From Au1		-1.95 eA-3
PLAT972_ALERT_2_C	Check	Calcd Resid. Dens.	0.71Ang	From Au3		-1.93 eA-3
PLAT972_ALERT_2_C	Check	Calcd Resid. Dens.	0.77Ang	From Au3		-1.76 eA-3
PLAT972_ALERT_2_C	Check	Calcd Resid. Dens.	0.88Ang	From Au3		-1.52 eA-3
PLAT972_ALERT_2_C	Check	Calcd Resid. Dens.	0.97Ang	From Au2		-1.52 eA-3
PLAT973_ALERT_2_C	Check	Calcd Positive Resid. Density on		Au1		1.48 eA-3
PLAT977_ALERT_2_C	Check	Negative Difference Density on H81		.		-0.32 eA-3
PLAT977_ALERT_2_C	Check	Negative Difference Density on H83		.		-0.35 eA-3

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3	Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H-Atoms	8	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	1	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	4	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0010	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar	0.0010	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0010	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar	0.0010	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0010	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0010	Report
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	!	Info
PLAT791_ALERT_4_G	Model has Chirality at C7 (Sohncke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C29 (Sohncke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C65 (Sohncke SpGr)	R	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	8	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !	
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL	2019/3	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
	0 0 1,		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	430	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	2	Note
	-2 0 5, 2 0 4,		
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.9	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check	
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	3.595	Note
	Predicted wR2: Based on SigI**2 4.74 or SHELX Weight 18.92		
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

0	ALERT level A	= Most likely a serious problem - resolve or explain
11	ALERT level B	= A potentially serious problem, consider carefully
35	ALERT level C	= Check. Ensure it is not caused by an omission or oversight
27	ALERT level G	= General information/check it is not something unexpected
1	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
43	ALERT type 2	Indicator that the structure model may be wrong or deficient
13	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.

Datablock a - ellipsoid plot

