

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: i17601

Bond precision: C-C = 0.0093 Å

Wavelength=0.71073

Cell: a=17.426(3) b=17.980(3) c=21.735(3)
 alpha=85.450(7) beta=89.570(7) gamma=88.868(8)
Temperature: 100 K

	Calculated	Reported
Volume	6787.1(19)	6787.5(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C46 H56 Au N8, 2(C2 F6 N O4 S2), 3(C H2 Cl2)	C46 H56 Au N8, 2(C2 F6 N O4 S2), 3(C H2 Cl2)
Sum formula	C53 H62 Au Cl6 F12 N10 O8 S4	C53 H62 Au Cl6 F12 N10 O8 S4
Mr	1733.04	1733.03
Dx, g cm ⁻³	1.696	1.696
Z	4	4
Mu (mm ⁻¹)	2.618	2.618
F000	3468.0	3468.0
F000'	3467.25	
h,k,lmax	22,23,28	22,23,27
Nref	30521	30276
Tmin,Tmax	0.598,0.592	0.570,0.746
Tmin'	0.587	

Correction method= # Reported T Limits: Tmin=0.570 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.992

Theta(max)= 27.293

R(reflections)= 0.0552(26631)

wR2(reflections)= 0.1553(30276)

S = 1.054

Npar= 1786

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

PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	4.1	Ratio
PLAT220_ALERT_2_C	Non-Solvent Resd 2 C	Ueq(max)/Ueq(min) Range	5.3	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference F6A_6	--C2A_6	0.17	Ang.
PLAT242_ALERT_2_C	Low 'MainMol'	Ueq as Compared to Neighbors of	S1_5	Check
PLAT242_ALERT_2_C	Low 'MainMol'	Ueq as Compared to Neighbors of	S2_5	Check
PLAT244_ALERT_4_C	Low 'Solvent'	Ueq as Compared to Neighbors of	C1_7	Check
PLAT244_ALERT_4_C	Low 'Solvent'	Ueq as Compared to Neighbors of	C1_10	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C11_7	0.110	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C11_10	0.106	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C11A_11	0.110	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C11_12	0.134	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C11B_11	0.110	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00926	Ang.
PLAT431_ALERT_2_C	Short Inter HL..A Contact F1_4	..O4A_6	2.88	Ang.
		x,y,z =	1_555	Check
PLAT431_ALERT_2_C	Short Inter HL..A Contact F2_4	..O4A_6	2.80	Ang.
		x,y,z =	1_555	Check
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #		1	Note
	C46 H56 Au N8			

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	51	Note	
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	17	Report	
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF		Please Check	
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	62.45	Why ?	
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	2	Units	
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	20	Report	
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report	
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	5	Report	
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	5	Report	
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3	Note	
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	5	Report	
PLAT242_ALERT_2_G	Low 'MainMol'	C1_3	Check	
PLAT242_ALERT_2_G	Low 'MainMol'	C2_3	Check	
PLAT242_ALERT_2_G	Low 'MainMol'	C1_4	Check	
PLAT242_ALERT_2_G	Low 'MainMol'	C2_4	Check	
PLAT242_ALERT_2_G	Low 'MainMol'	C1_5	Check	
PLAT242_ALERT_2_G	Low 'MainMol'	C2_5	Check	
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6)	100%	Note	
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 7)	100%	Note	
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 9)	100%	Note	
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 12)	100%	Note	
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 14)	100%	Note	
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 15)	100%	Note	
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 6	9.14	Check	
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 7	5.86	Check	
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 9	3.26	Check	
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 12	2.96	Check	
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 14	1.75	Check	
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 15	2.04	Check	
PLAT432_ALERT_2_G	Short Inter X...Y Contact F6A_6	..C36_2	2.95	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2_3	..C25_2	2.88	Ang.
		x,y,z =	1_555	Check

PLAT432_ALERT_2_G Short Inter X...Y Contact	O4_3	..C2_1	3.00 Ang.
		x,y,z =	1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	O3B_6	..C33_2	3.00 Ang.
		x,y,z =	1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact	Cl2_7	..Cl1B_8	2.79 Ang.
		x,y,z =	1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact	Cl1_9	..Cl2_10	3.26 Ang.
		-1+x,y,z =	1_455 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact	F2_4	..F5B_6	2.69 Ang.
		x,y,z =	1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels		337 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.	#		11 Note
	C H2 Cl2		
PLAT860_ALERT_3_G Number of Least-Squares Restraints		192 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary	.		Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File	...		26 Note

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 28 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
 24 ALERT type 4 Improvement, methodology, query or suggestion
 0 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 i17601 - ellipsoid plot

