

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) i18943

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: i18943

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Bond precision:      C-C = 0.0044 Å      Wavelength=0.71073

Cell:                      a=16.2506(9)      b=15.8856(9)      c=24.5298(14)  
                            alpha=90      beta=100.138(2)      gamma=90

Temperature:      100 K

	Calculated	Reported
Volume	6233.5(6)	6233.5(6)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C <sub>46</sub> H <sub>56</sub> Au N <sub>8</sub> , C <sub>2</sub> F <sub>6</sub> N O <sub>4</sub> S <sub>2</sub> , 2(C H <sub>2</sub> Cl <sub>2</sub> ) [+ solvent]	C <sub>46</sub> H <sub>56</sub> Au N <sub>8</sub> , 2(C H <sub>2</sub> Cl <sub>2</sub> ), C <sub>2</sub> F <sub>6</sub> N O <sub>4</sub> S <sub>2</sub> , 1.5[CH <sub>2</sub> CL <sub>2</sub> ]
Sum formula	C <sub>50</sub> H <sub>60</sub> Au Cl <sub>4</sub> F <sub>6</sub> N <sub>9</sub> O <sub>4</sub> S <sub>2</sub> [+ solvent]	C <sub>51.50</sub> H <sub>63</sub> Au Cl <sub>7</sub> F <sub>6</sub> N <sub>9</sub> O <sub>4</sub> S <sub>2</sub>
Mr	1367.96	1495.34
Dx, g cm <sup>-3</sup>	1.458	1.593
Z	4	4
Mu (mm <sup>-1</sup> )	2.663	2.795
F <sub>000</sub>	2752.0	3004.0
F <sub>000</sub> '	2748.51	
h, k, l <sub>max</sub>	20, 20, 31	20, 20, 31
N <sub>ref</sub>	6935	6925
T <sub>min</sub> , T <sub>max</sub>	0.450, 0.497	0.491, 0.746
T <sub>min</sub> '	0.416	

Correction method= # Reported T Limits: T<sub>min</sub>=0.491 T<sub>max</sub>=0.746

AbsCorr = MULTII-SCAN

Data completeness= 0.999

Theta(max)= 27.159

R(reflections)= 0.0281( 6692)

wR2(reflections)=  
0.0767( 6925)

S = 1.106

Npar= 427

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

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report  
PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.93Ang From Cl2A 1.97 eA-3



### Alert level G

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and the formula from the \_atom\_site\* data.  
Atom count from \_chemical\_formula\_sum: C51.5 H63 Au1 Cl7 F6 N9 O4 S2  
Atom count from the \_atom\_site data: C50 H60 Au1 Cl4 F6 N9 O4 S2  
CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
CELLZ01\_ALERT\_1\_G ALERT: Large difference may be due to a  
symmetry error - see SYMMG tests  
From the CIF: \_cell\_formula\_units\_Z 4  
From the CIF: \_chemical\_formula\_sum C51.50 H63 Au Cl7 F6 N9 O4 S2  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	206.00	200.00	6.00
H	252.00	240.00	12.00
Au	4.00	4.00	0.00
Cl	28.00	16.00	12.00
F	24.00	24.00	0.00
N	36.00	36.00	0.00
O	16.00	16.00	0.00
S	8.00	8.00	0.00

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 21 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 15 Report  
PLAT041\_ALERT\_1\_G Calc. and Reported SumFormula Strings Differ Please Check  
PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT051\_ALERT\_1\_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 4.71 %  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 24.98 Why ?  
PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 3 Report  
PLAT176\_ALERT\_4\_G The CIF-Embedded .res File Contains SADI Records 8 Report  
PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 1 Report  
PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0020 Report  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of S1 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of S2 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F1 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F2 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F3 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F4 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F5 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F6 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O1 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O2 Constrained at 0.5 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of O3	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O4	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N5	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C25	Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )		100%	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 2 )		7.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 3 )		3.58	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 4 )		1.42	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure		202	A**3
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		15	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....		!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		130	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed		!	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		8	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		2	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		5	Info

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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  
 2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 43 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 7 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 4 ALERT type 3 Indicator that the structure quality may be low  
 28 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.

