

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: 1008235

Bond precision:	C-C = 0.0080 Å	Wavelength=0.71073	
Cell:	a=11.5505(1) alpha=90	b=8.9467(1) beta=112.3919(6)	c=14.6047(2) gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1395.44(3)	1395.44(3)	
Space group	P 21/n	P 21/n	
Hall group	-P 2yn	?	
Moiety formula	C8 H13 Cl2 N O2 Pt S, O	?	
Sum formula	C8 H13 Cl2 N O3 Pt S	C8 H15 Cl2 N O3 Pt S	
Mr	469.24	471.26	
Dx, g cm-3	2.234	2.243	
Z	4	4	
Mu (mm-1)	10.579	10.579	
F000	880.0	888.0	
F000'	875.61		
h, k, lmax	15, 11, 18	14, 11, 18	
Nref	3194	3149	
Tmin, Tmax	0.433, 0.530	0.485, 0.569	
Tmin'	0.425		

Correction method= MULTI-SCAN

Data completeness= 0.986 Theta(max)= 27.490

R(reflections)= 0.0310(3027) wR2(reflections)= 0.0809(3149)

S = 1.135 Npar= Npar = 150

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

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)

01 Check

🟢 Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 2.02 Check

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check

🟠 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: C8 H15 Cl2 N1 O3 Pt1 S1

Atom count from the _atom_site data: C8 H13 Cl2 N1 O3 Pt1 S1

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?

From the CIF: _cell_formula_units_Z 4

From the CIF: _chemical_formula_sum C8 H15 Cl2 N1 O3 Pt1 S1

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	32.00	32.00	0.00
H	60.00	52.00	8.00
Cl	8.00	8.00	0.00
N	4.00	4.00	0.00
O	12.00	12.00	0.00
Pt	4.00	4.00	0.00
S	4.00	4.00	0.00

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Why ?

PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check

PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check

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

- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 2 ALERT type 2 Indicator that the structure model may be wrong or deficient
 - 0 ALERT type 3 Indicator that the structure quality may be low
 - 0 ALERT type 4 Improvement, methodology, query or suggestion
 - 2 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*, 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.

