**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: f8\_1\_fin1\_sq**

Bond precision:

C-C = 0.0103

A

Wavelength=0.71073

Cell:

a=33.591(7)

alpha=90

150 K

b=13.237(3)

beta=125.805(2)

c=24.401(9)

gamma=90

Temperature:

Calculated

8799(4) C 2/c

-C 2yc

Reported

8800(4) C 2/c

-C 2yc

?

Volume

Space group

Hall group

Moiety formula

C40

Cl3

C41

H34

As2

Au2

Cl2

O4, C

H

[+ solvent]

H35 As2

Au2

Cl5

O4

[+

Sum formula

Mr

C41 H35 As2 Au2 Cl5 O4

1312.72

1.982

8

8.497

4976.0

solvent]

1312.72

1.982

8

8.497

4976.0

4953.98

44,17,32

10636

0.306,0.428

0.191

Dx,g

Z

cm-3

Mu (mm-1) F000

F000’ h,k,lmax Nref Tmin,Tmax Tmin’

44,17,32

10614

0.239,0.746

Correction

method= # Reported

T

Limits: Tmin=0.239 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta(max)= 27.998

wR2(reflections)=

0.0952( 10614)

R(reflections)= 0.0378( 8434)

S = 0.992

Npar= 489

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**

PLAT213\_ALERT\_2\_C PLAT213\_ALERT\_2\_C PLAT220\_ALERT\_2\_C PLAT222\_ALERT\_3\_C PLAT241\_ALERT\_2\_C PLAT241\_ALERT\_2\_C PLAT244\_ALERT\_4\_C PLAT342\_ALERT\_3\_C PLAT413\_ALERT\_2\_C

Atom O1B Atom C8B NonSolvent NonSolvent

has has

Resd 1 C

ADP max/min Ratio ADP max/min Ratio Ueq(max)/Ueq(min)

.....

..... Range Range

3.5

3.1

5.0

4.5

O1A O1B C100

0.01026

2.10

prolat prolat Ratio Ratio Check Check Check Ang. Ang.

Resd 1 H

Uiso(max)/Uiso(min)

High High Low

’MainMol’

’MainMol’

’Solvent’

Ueq Ueq Ueq

as as as

Compared Compared Compared

to to to

Neighbors Neighbors Neighbors

of of of

Low Bond Precision on C-C Bonds

...............

Short Inter XH3 .. XHn

H5B

..H20B

.

x,1-y,-1/2+z

=

6\_565 Check

**Alert level** PLAT128\_ALERT\_4\_G PLAT434\_ALERT\_2\_G

**G**

Alternate Setting for Input Space Group

C2/c

I2/a Note

3.39 Ang.

4\_545 Check

3.27 Ang.

Short Inter HL..HL Contact Cl1

..Cl11

1/2-x,-1/2+y,1/2-z

=

PLAT434\_ALERT\_2\_G

Short Inter HL..HL Contact Cl10

..Cl10

1/2-x,3/2-y,-z

=

7\_565

Check

PLAT605\_ALERT\_4\_G PLAT869\_ALERT\_4\_G PLAT883\_ALERT\_1\_G PLAT941\_ALERT\_3\_G PLAT967\_ALERT\_5\_G

Largest Solvent Accessible VOID in the Structure ALERTS Related to the Use of SQUEEZE Suppressed No Info/Value for \_atom\_sites\_solution\_primary . Average HKL Measurement Multiplicity ........... Note: Two-Theta Cutoff Value in Embedded .res ..

168

! Please

3.7

56.0

A\*\*3

Info Do ! Low Degree

0

0

9

8

**ALERT ALERT ALERT ALERT**

**level level level level**

**A B C G**

=

=

=

=

Most likely a A potentially Check. Ensure

serious problem - resolve or explain serious problem, consider carefully

it is not caused by an omission or oversight

General information/check it is not something unexpected

1

8

3

4

1

ALERT ALERT ALERT ALERT ALERT

type type type type type

1

2

3

4

5

CIF construction/syntax error, inconsistent or missing data Indicator that the structure model may be wrong or deficient Indicator that the structure quality may be low

Improvement, methodology, query or suggestion

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.

**PLATON version of 18/12/2021; check.def file version of 18/12/2021Datablock f8\_1\_fin1\_sq** - ellipsoid plot

**Datablock f8\_1\_fin1\_sq** - ellipsoid plot

