

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo\_Wenzel\_SW663\_0m\_a\_sq

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: mo\_Wenzel\_SW663\_0m\_a\_sq

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Bond precision:      C-C = 0.0067 Å      Wavelength=0.71073

Cell:                      a=19.9908 (5)      b=19.9908 (5)      c=19.9908 (5)  
                                    alpha=90      beta=90      gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	7989.0 (6)	7989.0 (6)
Space group	I -4 3 d	I -4 3 d
Hall group	I -4bd 2c 3	I -4bd 2c 3
Moiety formula	C36 F4 Ga3 O24 [+ solvent]	?
Sum formula	C36 F4 Ga3 O24 [+ solvent]	C36 H8 F4 Ga3 O24
Mr	1101.51	1109.60
Dx, g cm <sup>-3</sup>	0.916	0.916
Z	4	4
Mu (mm <sup>-1</sup> )	1.061	1.061
F000	2148.0	2148.0
F000'	2152.15	
h, k, lmax	26, 26, 26	26, 26, 26
Nref	1664 [ 901]	1662
Tmin, Tmax	0.767, 0.767	0.682, 0.746
Tmin'	0.751	

Correction method= # Reported T Limits: Tmin=0.682 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 1.84/1.00      Theta(max)= 28.273

R(reflections)= 0.0260 ( 1396)

wR2(reflections)=  
0.0909 ( 1662)

S = 1.092

Npar= 57

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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.

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**Alert level B**

PLAT987\_ALERT\_1\_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

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**Alert level C**

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C3 Check  
PLAT250\_ALERT\_2\_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.7 Note  
PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including Ga1 0.133 Check  
PLAT341\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00667 Ang.  
PLAT934\_ALERT\_3\_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check  
0 2 6,

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**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:C36 H8 F4 Ga3 O24  
Atom count from the \_atom\_site data: C36 F4.0046 Ga3 O24

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 C36 H8 F4 Ga3 O24  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	144.00	144.00	0.00
H	32.00	0.00	32.00
F	16.00	16.00	0.00
Ga	12.00	12.00	0.00
O	96.00	96.00	0.00

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 3 Info  
PLAT040\_ALERT\_1\_G No H-atoms in this Carbon Containing Compound .. Please Check  
PLAT041\_ALERT\_1\_G Calc. and Reported SumFormula Strings Differ Please Check  
Calc: C36 F4 Ga3 O24  
Rep.: C36 H8 F4 Ga3 O24

PLAT300\_ALERT\_4\_G Atom Site Occupancy of F1 Constrained at 0.3333 Check  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1) 6% Note  
PLAT606\_ALERT\_4\_G Solvent Accessible VOID(S) in Structure ..... ! Info  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Ga1 (III) . 2.94 Info  
PLAT869\_ALERT\_4\_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 8.518 Note  
Predicted wR2: Based on SigI\*\*2 1.07 or SHELX Weight 8.41  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 0 Info

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

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

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**PLATON version of 22/08/2024; check.def file version of 21/08/2024**

