

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

**Datablock: sw231**

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Bond precision:	C-C = 0.0300 A	Wavelength=1.54178	
Cell:	a=18.59063(18)	b=18.59063(18)	c=10.20330(9)
	alpha=90	beta=90	gamma=120
Temperature:	100 K		
	Calculated	Reported	
Volume	3053.93(5)	3053.93(4)	
Space group	P 63/m	P 63/m	
Hall group	-P 6c	-P 6c	
Moiety formula	C12 Al F27 O3, 3(C7 H5 Mo O2 P3), C4 F9, 0.34(O3), In	C16 AL F36 O4, 3(C7 H5 MO O2 P3), IN	
Sum formula	C37 H15 Al F36 In Mo3 O10.02 P9	C37 H15 Al F36 In Mo3 O10 P9	
Mr	2012.16	2012.16	
Dx,g cm-3	2.188	2.188	
Z	2	2	
Mu (mm-1)	11.804	11.804	
F000	1928.0	1928.0	
F000'	1941.49		
h,k,lmax	22,22,12	22,20,12	
Nref	1916	1903	
Tmin,Tmax	0.354,0.433	0.025,0.775	
Tmin'	0.000		

Correction method= GAUSSIAN

Data completeness= 0.993      Theta(max)= 66.590

R(reflections)= 0.0907( 1812)      wR2(reflections)= 0.2045( 1903)

S = 1.164      Npar= 243

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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 A

PLAT242_ALERT_2_A Check Low	Ueq as Compared to Neighbors for	All
PLAT307_ALERT_2_A Isolated Metal Atom (Unusual !)	.....	In1
PLAT431_ALERT_2_A Short Inter HL..A Contact	F7A .. F9A ..	1.86 Ang.

PLAT431_ALERT_2_A	Short Inter HL..A Contact	F7C	..	F9A	..	2.08	Ang.
PLAT431_ALERT_2_A	Short Inter HL..A Contact	F9A	..	O3	..	2.08	Ang.
PLAT432_ALERT_2_A	Short Inter X...Y Contact	F7A	..	C9A	..	2.63	Ang.
PLAT432_ALERT_2_A	Short Inter X...Y Contact	F9A	..	C7	..	1.93	Ang.
PLAT432_ALERT_2_A	Short Inter X...Y Contact	F9A	..	C6	..	2.25	Ang.
PLAT432_ALERT_2_A	Short Inter X...Y Contact	C6	..	O3	..	1.17	Ang.
PLAT432_ALERT_2_A	Short Inter X...Y Contact	C6	..	O3	..	1.17	Ang.
PLAT432_ALERT_2_A	Short Inter X...Y Contact	C6	..	O3	..	1.17	Ang.
PLAT432_ALERT_2_A	Short Inter X...Y Contact	C7	..	O3	..	2.29	Ang.

### Alert level B

CRYSS02\_ALERT\_3\_B The value of \_exptl\_crystal\_size\_max is > 1.0  
Maximum crystal size given = 1.016

PLAT088_ALERT_3_B	Poor Data / Parameter Ratio .....	7.83
PLAT241_ALERT_2_B	Check High Ueq as Compared to Neighbors for	C4
PLAT242_ALERT_2_B	Check Low Ueq as Compared to Neighbors for	C9B
PLAT242_ALERT_2_B	Check Low Ueq as Compared to Neighbors for	Mo1
PLAT242_ALERT_2_B	Check Low Ueq as Compared to Neighbors for	C7
PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds (x 1000) Ang ..	30
PLAT431_ALERT_2_B	Short Inter HL..A Contact F7A .. F9C ..	2.50 Ang.
PLAT431_ALERT_2_B	Short Inter HL..A Contact F7C .. F9B ..	2.53 Ang.
PLAT431_ALERT_2_B	Short Inter HL..A Contact F7C .. F10A ..	2.58 Ang.
PLAT432_ALERT_2_B	Short Inter X...Y Contact F7C .. C9A ..	2.85 Ang.
PLAT432_ALERT_2_B	Short Inter X...Y Contact C7 .. C9A ..	3.08 Ang.

### Alert level C

PLAT215_ALERT_3_C	Disordered F9A has ADP max/min Ratio .....	3.40
PLAT241_ALERT_2_C	Check High Ueq as Compared to Neighbors for	C3
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for	F9D
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for	C8
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for	C2
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C3 - C3_a ...	1.53 Ang.
PLAT431_ALERT_2_C	Short Inter HL..A Contact F7C .. O3 ..	2.86 Ang.
PLAT432_ALERT_2_C	Short Inter X...Y Contact O2 .. C5 ..	2.96 Ang.
PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ	?
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	?
PLAT141_ALERT_4_C	su on a - Axis Small or Missing (x 100000) .....	18 Ang.
PLAT143_ALERT_4_C	su on c - Axis Small or Missing (x 100000) .....	9 Ang.
PLAT951_ALERT_1_C	Reported and Calculated Kmax Values Differ by ..	2

### 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: C37 H15 Al1 F36 In1 Mo3 O10 P9  
Atom count from the \_atom\_site data: C37 H15 Al1 F36 In1 Mo3 O10.02

REFLT03\_ALERT\_1\_G ALERT: Expected hkl max differ from CIF values

From the CIF: _diffrn_reflms_theta_max	66.59
From the CIF: _reflms_number_total	1903
From the CIF: _diffrn_reflms_limit_max hkl	22. 17. 12.
From the CIF: _diffrn_reflms_limit_min hkl	-21. -20. -12.
TEST1: Expected hkl limits for theta max	
Calculated maximum hkl	22. 22. 12.
Calculated minimum hkl	-22. -22. -12.

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	66.93
PLAT301_ALERT_3_G	Note: Main Residue Disorder .....	37.00 Perc.
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints .....	113
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size ....	1.02 mm
PLAT302_ALERT_4_G	Note: Anion/Solvent Disorder .....	13.00 Perc.

P1  
P2  
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12 ALERT level A = In general: serious problem
12 ALERT level B = Potentially serious problem
13 ALERT level C = Check and explain
10 ALERT level G = General alerts; check

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

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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.

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

Datablock sw231 - ellipsoid plot

