

# 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.

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**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.

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**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

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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`: 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:	<code>_diffrn_reflths_theta_max</code>	66.59
From the CIF:	<code>_reflths_number_total</code>	1903
From the CIF:	<code>_diffrn_reflths_limit_max</code> hkl	22. 17. 12.
From the CIF:	<code>_diffrn_reflths_limit_min</code> 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.

