

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo\_Wenzel\_SW735\_0ma\_a\_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\_SW735\_0ma\_a\_a\_sq

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

Cell:                      a=12.0022 (11)      b=13.1723 (12)      c=27.801 (2)  
                                    alpha=90                      beta=92.847 (3)      gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	4389.8 (6)	4389.8 (7)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C18 H2 Co F2 O15 Zn2 [+ solvent]	?
Sum formula	C18 H2 Co F2 O15 Zn2 [+ solvent]	C30 H31 Co F2 O15 Zn2
Mr	685.91	85923.00
Dx, g cm <sup>-3</sup>	1.038	1.038
Z	4	4
Mu (mm <sup>-1</sup> )	1.506	1.506
F000	1340.0	1340.0
F000'	1344.51	
h, k, lmax	16, 17, 37	16, 17, 37
Nref	11221	11160
Tmin, Tmax	0.633, 0.798	0.623, 0.746
Tmin'	0.621	

Correction method= # Reported T Limits: Tmin=0.623 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.995

Theta (max)= 28.599

R(reflections)= 0.0718( 8447)

wR2(reflections)=  
0.3036( 11160)

S = 1.304

Npar= 363

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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

TYPE017\_ALERT\_1\_A \_chemical\_formula\_weight is not data type numb.

DENSD01\_ALERT\_1\_A The ratio of the submitted crystal density and that  
calculated from the formula is outside the range 0.90 <> 1.10

Crystal density given = 1.038

Calculated crystal density = 1.300

SHFSU01\_ALERT\_2\_A The absolute value of parameter shift to su ratio > 0.20

Absolute value of the parameter shift to su ratio given 0.405

Additional refinement cycles may be required.

PLAT046\_ALERT\_1\_A Reported Z, MW and D(calc) are Inconsistent .... 130.010 Check

PLAT080\_ALERT\_2\_A Maximum Shift/Error ..... 0.41 Why ?

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### Alert level B

PLAT934\_ALERT\_3\_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 6 Check  
0 3 1, -2 0 2, 3 0 3, 2 2 3, -1 3 3, -7 2 7,

PLAT973\_ALERT\_2\_B Check Calcd Positive Resid. Density on Col 1.61 eA-3

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### Alert level C

PLAT084\_ALERT\_3\_C High wR2 Value (i.e. > 0.25) ..... 0.30 Report

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference F2A --C18 . 0.16 Ang.

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 01 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 03 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 04 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 07 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 08 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Zn1 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Zn2 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Co1 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C11 Check

PLAT341\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00667 Ang.

PLAT767\_ALERT\_4\_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check

PLAT905\_ALERT\_3\_C Negative K value in the Analysis of Variance ... -2.155 Report

PLAT918\_ALERT\_3\_C Reflection(s) with I(obs) much Smaller I(calc) . 4 Check

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 1.11Ang From O13 2.08 eA-3

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 1.15Ang From O15 1.74 eA-3

PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 1.09Ang From O6 . 0.72 eA-3

PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 1.03Ang From O14 . 0.54 eA-3

PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.67Ang From O6 . -0.51 eA-3

PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.99Ang From O14 . -0.46 eA-3

PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.85Ang From O14 . -0.41 eA-3

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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: C30 H31 Co1 F2 O15 Zn2  
 Atom count from the \_atom\_site data: C18 H2 Co1 F2 O15 Zn2  
 CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
 CELLZ01\_ALERT\_1\_G ALERT: Large difference may be due to a  
 symmetry error - see SYMMG tests  
 From the CIF: \_cell\_formula\_units\_Z 4  
 From the CIF: \_chemical\_formula\_sum C30 H31 Co F2 O15 Zn2  
 TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	120.00	72.00	48.00
H	124.00	8.00	116.00
Co	4.00	4.00	0.00
F	8.00	8.00	0.00
O	60.00	60.00	0.00
Zn	8.00	8.00	0.00

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 3 Info  
 PLAT041\_ALERT\_1\_G Calc. and Reported SumFormula Strings Differ Please Check  
 Calc: C18 H2 Co F2 O15 Zn2  
 Rep.: C30 H31 Co F2 O15 Zn2  
 PLAT230\_ALERT\_2\_G Hirshfeld Test Diff for F1B --C5 . 5.9 s.u.  
 PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Zn2 --O6\_f . 5.5 s.u.  
 PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Co1 --O13 . 5.3 s.u.  
 PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1) 5% Note  
 PLAT606\_ALERT\_4\_G Solvent Accessible VOID(S) in Structure ..... ! Info  
 PLAT794\_ALERT\_5\_G Tentative Bond Valency for Zn1 (II) . 2.19 Info  
 PLAT794\_ALERT\_5\_G Tentative Bond Valency for Zn2 (II) . 2.06 Info  
 PLAT794\_ALERT\_5\_G Tentative Bond Valency for Co1 (II) . 2.12 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 !  
 PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note  
 -1 0 1, 0 1 1, 0 0 2,  
 PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 57 Note  
 PLAT965\_ALERT\_2\_G The SHELXL WEIGHT Optimisation has not Converged Please Check  
 PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 13.116 Note  
 Predicted wR2: Based on SigI\*\*2 2.31 or SHELX Weight 23.49  
 PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 0 Info

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

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

Datablock mo\_Wenzel\_SW735\_0ma\_a\_a\_sq - ellipsoid plot

