



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mils028

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: mils028

Bond precision: C-C = 0.0033 Å

Wavelength=1.54178

Cell: a=12.9852 (3) b=13.0369 (3) c=25.3459 (6)
 alpha=101.905 (1) beta=90.031 (1) gamma=90.023 (1)
Temperature: 200 K

	Calculated	Reported
Volume	4198.44 (17)	4198.43 (17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C86 H74 Co N6, C16 H32 Li O4	C86 H74 Co N6, C16 H32 Li O4
Sum formula	C102 H106 Co Li N6 O4	C102 H106 Co Li N6 O4
Mr	1545.80	1545.79
Dx, g cm ⁻³	1.223	1.223
Z	2	2
Mu (mm ⁻¹)	2.044	2.044
F000	1644.0	1644.0
F000'	1643.49	
h, k, lmax	16, 16, 31	16, 16, 31
Nref	17223	16385
Tmin, Tmax	0.664, 0.779	0.622, 0.754
Tmin'	0.587	

Correction method= # Reported T Limits: Tmin=0.622 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.951

Theta(max)= 74.624

R(reflections)= 0.0487(14330)

wR2(reflections)=
0.1232(16385)

S = 1.050

Npar= 1039

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**

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	3.3	Ratio
PLAT911_ALERT_3_C	Missing FCF	Refl	Between	Thmin & STh/L=	0.600	261	Report
	12 9 0,	11 10 0,	10 11 0,	-3-15 1,	-2-15 1,	-1-15 1,	
	0-15 1,	-10-11 1,	-11-10 1,	-12 -9 1,	-2 -3 1,	3 -2 1,	
	-14 6 1,	-13 8 1,	4 14 1,	-3-15 2,	-2-15 2,	-1-15 2,	
	0-15 2,	1-15 2,	-11-10 2,	-12 -9 2,	0 -4 2,	-15 -2 2,	
	3 -2 2,	-15 -1 2,	0 -1 2,	-15 0 2,	0 0 2,	-14 5 2,	
	(231 More NOT listed: see .ckf listing file)						

● **Alert level G**

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001	Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Col --N1 .	5.2	s.u.
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C75	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Col (III) .	3.65	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	574	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	3	Note
	-2 -3 1, 3 -2 1, 3 -2 2,		
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	6	Note
	-2 -3 1, 0 -1 2, 0 0 2, 1 -2 5, 3 -2 1,	3 -2 2,	
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.0	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	2.958	Note
	Predicted wR2: Based on SigI**2 4.16 or SHELX Weight 11.73		
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info
PLAT994_ALERT_1_G	SHELXL .ins Contains no or MERG 0 Instruction ..	!	Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 15/01/2026; check.def file version of 02/01/2026

Datablock mlls028 - ellipsoid plot

