

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:	C-C = 0.0060 A	Wavelength=0.71073
Cell:	a=25.681(3) b=8.9889(9) c=18.4468(18)	
	alpha=90 beta=133.511(6) gamma=90	
Temperature:	293 K	
	Calculated	Reported
Volume	3088.3(6)	3088.3(6)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C24 H52 Cl Cr Li2 O6	C24 H52 Cl Cr Li2 O6
Sum formula	C24 H52 Cl Cr Li2 O6	C24 H52 Cl Cr Li2 O6
Mr	537.99	537.98
Dx,g cm-3	1.157	1.157
Z	4	4
Mu (mm-1)	0.488	0.488
F000	1164.0	1164.0
F000'	1166.32	
h,k,lmax	32,11,23	32,11,23
Nref	3296	3256
Tmin,Tmax	0.943,0.952	0.913,0.986
Tmin'	0.907	

Correction method= # Reported T Limits: Tmin=0.913 Tmax=0.986
AbsCorr = NUMERICAL

Data completeness= 0.988 Theta(max)= 26.781

R(reflections)= 0.0462(1405) wR2(reflections)= 0.1054(3256)

S = 0.778 Npar= 158

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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as numerical

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00
Goodness of fit given = 0.778

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.143

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 43% Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C13 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C1 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.209 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 10 Report

PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

● Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info

PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 0.143 Report

PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a Note

PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check

PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check

PLAT794_ALERT_5_G Tentative Bond Valency for Cr1 (III) . 2.72 Info

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 31 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

7 **ALERT level G** = General information/check it is not something unexpected

3 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

5 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. 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.

