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

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Bond precision:  C-C = 0.0108 A          Wavelength=0.71073

Cell:           a=14.8499(6)    b=10.7574(5)       c=22.6334(11)
                alpha=90        beta=90.059(4)     gamma=90
Temperature:    293 K

                Calculated                Reported
Volume          3615.6(3)                 3615.6(3)
Space group     P 21/c                    P 21/c
Hall group      : -P 2ybc                 -P 2ybc
Moiety formula  C32 H44 Cr F6 Li N2 O6    C32 H44 Cr F6 Li N2 O6
Sum formula     C32 H44 Cr F6 Li N2 O6    C32 H44 Cr F6 Li N2 O6
Mr              725.63                    725.63
Dx,g cm-3       1.333                     1.333
Z               4                         4
Mu (mm-1)       0.390                     0.390
F000            1516.0                    1516.0
F000'           1518.21
h,k,lmax        18,13,28                  18,13,28
Nref            7768                      7685
Tmin,Tmax       0.911,0.925               0.830,0.961
Tmin'           0.890

Correction method= # Reported T Limits: Tmin=0.830 Tmax=0.961
AbsCorr = NUMERICAL

Data completeness= 0.989          Theta(max)= 26.845

R(reflections)= 0.0679( 4816)     wR2(reflections)= 0.1826( 7685)

S = 1.040                 Npar= 435
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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.

Alert level C

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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
PLAT213_ALERT_2_C Atom F4             has ADP max/min Ratio .....        3.2 prolat
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C16 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C29 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C32 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C9 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C31 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01085 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C29      - C31      .       1.43 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.055 Check
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Alert level G

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PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of         C2 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C22 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cr1       (III)     .       3.05 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         82 Note
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 0 0 1)         Est.d BASF       0.46 Check
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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. 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.

PLATON version of 19/10/2018; check.def file version of 15/10/2018

Datablock shelx - ellipsoid plot