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 = 0.0113 A          Wavelength=0.71073

Cell:           a=53.4099(19)    b=9.1895(3)       c=17.9050(6)
                alpha=90         beta=99.190(2)    gamma=90
Temperature:    150 K

                Calculated                Reported
Volume          8675.2(5)                 8675.2(5)
Space group     C 2                       C 2
Hall group      C 2y                      C 2y
Moiety formula  C32 H20 F6 O6 Ti          C32 H20 F6 O6 Ti
Sum formula     C32 H20 F6 O6 Ti          C32 H20 F6 O6 Ti
Mr              662.35                    662.38
Dx,g cm-3       1.521                     1.521
Z               12                        12
Mu (mm-1)       0.380                     0.380
F000            4032.0                    4032.0
F000'           4038.15
h,k,lmax        66,11,22                  66,11,22
Nref            17757[ 9458]              17751
Tmin,Tmax       0.910,0.925               0.680,0.746
Tmin'           0.857

Correction method= # Reported T Limits: Tmin=0.680 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.88/1.00      Theta(max)= 26.373

R(reflections)= 0.0729( 12859)    wR2(reflections)= 0.1947( 17751)

S = 1.026                 Npar= 1217
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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 A

PLAT213_ALERT_2_A Atom F10 has ADP max/min Ratio ..... 5.4 prolat
PLAT213_ALERT_2_A Atom F11 has ADP max/min Ratio ..... 5.2 prolat

Alert level B

PLAT213_ALERT_2_B Atom F2 has ADP max/min Ratio ..... 4.5 prolat
PLAT213_ALERT_2_B Atom F5 has ADP max/min Ratio ..... 4.2 prolat
PLAT213_ALERT_2_B Atom F9 has ADP max/min Ratio ..... 4.4 prolat
PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.500
From the CIF: _refine_ls_abs_structure_Flack_su 0.000
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 7.77 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.19 Report
PLAT213_ALERT_2_C Atom F1 has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom F3 has ADP max/min Ratio ..... 3.8 prolat
PLAT213_ALERT_2_C Atom F8 has ADP max/min Ratio ..... 3.8 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 F Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference F1 -- C13 .. 0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C86 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01133 Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min) 6 Note
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density 0 Note

Alert level G

PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.500 Note
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.52 Why ?
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C13 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C20 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C45 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C52 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C74 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C90 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F3 .. F6 .. 2.70 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F7 .. F12 .. 2.71 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F8 .. F10 .. 2.82 Ang.
PLAT916_ALERT_2_G Hooft y and Flack x Parameter values differ by . 0.14 Check
PLAT916_ALERT_2_G Hooft y and Flack x Parameter values differ by . 0.14 Check

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

1 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
3 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
0 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 30/03/2016; check.def file version of 30/03/2016

Datablock shelx - ellipsoid plot