

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 = 0.0078 A Wavelength=0.71073

Cell: a=38.492(6) b=20.574(11) c=21.340(13)
 alpha=90 beta=90 gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	16900(14)	16900(14)
Space group	P c c n	P c c n
Hall group	-P 2ab 2ac	-P 2ab 2ac
Moiety formula	C80 H48 F24 O20 Ti4	C80 H48 F24 O20 Ti4
Sum formula	C80 H48 F24 O20 Ti4	C80 H48 F24 O20 Ti4
Mr	1976.67	1976.78
Dx,g cm-3	1.554	1.554
Z	8	8
Mu (mm-1)	0.486	0.486
F000	7936.0	7936.0
F000'	7951.14	
h,k,lmax	46,24,25	46,24,25
Nref	15486	15473
Tmin,Tmax	0.900,0.936	0.756,0.801
Tmin'	0.885	

Correction method= # Reported T Limits: Tmin=0.756 Tmax=0.801
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.349

R(reflections)= 0.0726(10763) wR2(reflections)= 0.1706(15473)

S = 1.080 Npar= 1153

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 B

PLAT213_ALERT_2_B Atom F18 has ADP max/min Ratio 4.8 prolat
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min) 11 Note

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.127
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 0.127 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.04 Report
PLAT213_ALERT_2_C Atom F14 has ADP max/min Ratio 3.1 prolat
PLAT213_ALERT_2_C Atom F15 has ADP max/min Ratio 3.8 prolat
PLAT213_ALERT_2_C Atom F17 has ADP max/min Ratio 3.6 prolat
PLAT213_ALERT_2_C Atom C57 has ADP max/min Ratio 3.2 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1 F Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for F18 -- C80 .. 5.5 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference F17 -- C80 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C42 -- C43 .. 0.17 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C43 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C24 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00781 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 92 Ang3
PLAT906_ALERT_2_C Large K value in the Analysis of Variance 11.817 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.599 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 2 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density 0 Note

Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 46.25 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ti1 -- O17 .. 5.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ti2 -- O17 .. 7.4 s.u.
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C31 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C38 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 C59 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C66 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C73 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C80 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
20 **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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
24 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
2 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.

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