checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FPR867B

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: FPR867B

Bond precision: C-C = 0.0240 A Wavelength=0.71073

Cell: a=12.2906(17) b=17.962(3) c=18.439(3)
alpha=90.015(5) beta=99.337(5) gamma=100.196(5)
Temperature: 150 K

	Calculated	Reported
Volume	3951.5(11)	3951.7(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C64 H26 F36 N4 O12 Yb2, C6 H14	C70 H40 F36 N4 O12 Yb2
Sum formula	C70 H40 F36 N4 O12 Yb2	C70 H40 F36 N4 O12 Yb2
Mr	2159.14	2159.14
Dx,g cm-3	1.815	1.815
Z	2	2
Mu (mm-1)	2.498	2.498
F000	2096.0	2096.0
F000’	2096.22	
h,k,lmax	15,23,23	15,23,23
Nref	18103	17903
Tmin,Tmax	0.507,0.638	0.557,0.638
Tmin’	0.456	

Correction method= # Reported T Limits: Tmin=0.557 Tmax=0.638
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 27.485

R(reflections)= 0.1070(14464) wR2(reflections)= 0.2787(17903)

S = 1.076 Npar= 1025

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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.93A From Yb2 10.81 eA-3
PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.87A From Yb1 4.34 eA-3
PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.68A From Yb2 -3.84 eA-3
PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Yb1 2.79 eA-3

Alert level B

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 11.27 eA-3
PLAT213_ALERT_2_B Atom F35 has ADP max/min Ratio ..... 4.9 prolat
PLAT230_ALERT_2_B Hirshfeld Test Diff for F25 --C55 . 7.8 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for F27 --C55 . 16.2 s.u.
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02402 Ang.
PLAT434_ALERT_2_B Short Inter HL..HL Contact F25 ..F24B 2.35 Ang.
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 24 Note
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 2 Check
PLAT939_ALERT_3_B Large Value of Not (SHELXL) Weight Optimized S . 148.49 Check
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.37A From O3 2.83 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.60A From Yb2 -3.34 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.02A From Yb1 -3.10 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 2.00A From F15 -2.94 eA-3

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.28 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.80 Report
PLAT213_ALERT_2_C Atom F7 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom F17 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom F19 has ADP max/min Ratio ..... 3.7 prolat
PLAT213_ALERT_2_C Atom F31 has ADP max/min Ratio ..... 3.8 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.7 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1 F Ueq(max)/Ueq(min) Range 4.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for F28 --C59 . 5.2 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference F22 --C54 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F26 --C55 0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F34 --C64 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F22B --C54 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F24B --C54 0.25 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C62 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.0 Note
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C65 - C66 . 1.42 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C67 - C68 . 1.43 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C68 - C69 . 1.43 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.713 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 158 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 3 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.11A From F14 2.28 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.73A From F2 2.17 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.90A From Yb2 2.12 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.36A From Yb1 2.08 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.05A From Yb1 1.91 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.52A From F25 1.70 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.12A From F15 1.64 eA-3

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.07A   From F26            1.59 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.21A   From O6            -2.28 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.08A   From C55           -2.09 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.91A   From Yb1           -2.09 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.81A   From Yb1           -1.92 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.89A   From Yb1           -1.82 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.04A   From Yb1           -1.78 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.33A   From O11           -1.69 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.88A   From Yb1           -1.65 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.00A   From Yb1           -1.64 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.19A   From O11           -1.51 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H26             -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H70A            -0.45 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.         0 Info
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        11 Note
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0     0.998 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ  Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large  116.02 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.005 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         5 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         5 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for   F23      --C54       .       6.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   F24      --C54       .       5.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   F23B     --C54       .       6.0 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C35 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C39 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C40 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C44 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       C49 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C50 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C54 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C55 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       C60 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C64 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        3% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  C21      ..C70            3.18 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C26      ..C26            3.18 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F25      ..F35            2.80 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F29      ..F29            2.63 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Yb1       (III)     .      3.32 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Yb2       (III)     .      3.39 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        12 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        18 Note
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  4 ALERT level A = Most likely a serious problem - resolve or explain
 13 ALERT level B = A potentially serious problem, consider carefully
 45 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 31 ALERT level G = General information/check it is not something unexpected

  4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 69 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 ALERT type 3 Indicator that the structure quality may be low
  8 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
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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 23/04/2018; check.def file version of 23/04/2018

Datablock FPR867B - ellipsoid plot