checkCIF/PLATON report

Structure factors have been supplied for datablock(s) K0705

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: K0705

Bond precision: C-C = 0.0248 A   Wavelength=0.71073

Cell: a=10.321(3)   b=15.231(4)   c=15.663(4)
               alpha=82.730(6)   beta=80.201(5)   gamma=71.847(6)
Temperature: 293 K

	Calculated	Reported
Volume	2298.4(11)	2298.5(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C6 F12 I2, 2(C18 H27 P)	2(C18 H27 P), (C6 F12 I2)
Sum formula	C42 H54 F12 I2 P2	C42 H54 F12 I2 P2
Mr	1102.59	1102.59
Dx,g cm-3	1.593	1.593
Z	2	2
Mu (mm-1)	1.515	1.515
F000	1100.0	1100.0
F000'	1099.14	
h,k,lmax	11,16,17	11,16,17
Nref	6623	6489
Tmin,Tmax	0.843,0.930	0.604,0.745
Tmin'	0.827	

Correction method= # Reported T Limits: Tmin=0.604 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.980   Theta(max)= 23.278

R(reflections)= 0.1226(3224)   wR2(reflections)= 0.1922(6489)

S = 1.080   Npar= 605

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**
PLAT431_ALERT_2_A Short Inter HL..A Contact I1   ..P1   .   3.09 Ang.
                                                    x,y,z =   1_555 Check

Author Response: This contact is in keeping with similar reports in the literature.

🟠 **Alert level B**
THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
            Calculated sin(theta_max)/wavelength =   0.5560

Author Response: This crystal was weakly diffracting, especially at higher angles, thus no useful data was observed beyond this limit. It is worth noting that this was the best crystal examined from multiple attempts to grow good quality crystals.

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ....   0.02485 Ang.

Author Response: This is a result of the poor crystal quality, weak diffraction and significant disorder surrounding the fluoroalkyl chains. Despite this, the data and structural model are of significant use in displaying the connectivity of the components of the crystal and their packing arrangements. Furthermore, the bond precision between smaller atoms is secondary as the primary feature of this structure is the P-I interaction, the characteristics of which are reliable given that these are the heaviest elements in the structure.

🟡 **Alert level C**
PLAT082_ALERT_2_C High R1 Value ....   0.12 Report
PLAT213_ALERT_2_C Atom F1   has ADP max/min Ratio .....   3.1 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference F1   --C1   .   0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F2   --C1   .   0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C31   --C32   .   0.22 Ang.
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C1 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C2 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   2.7 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   I2B   0.108 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   I2A   0.107 Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H38A   ..I2A   .   3.33 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H42A   ..I2A   .   3.28 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ...... 16.298 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   2.730 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   4.904 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   2.957 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.556   134 Report
PLAT977_ALERT_2_C Check Negative Difference Density on H35B   -0.34 eA-3

⬤ Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        30 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        12 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ   Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    37.98 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records         1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         1 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records         2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         9 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)       293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  2  )      100% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  3  )      100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )     10.62 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )      9.38 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F4       ..F7B            2.81 Ang.
                                             1+x,y,z  =       1_655 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F6       ..F11A           2.76 Ang.
                                             1+x,y,z  =       1_655 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       259 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.0 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        0 Info
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 1 ALERT level A = Most likely a serious problem - resolve or explain
 2 ALERT level B = A potentially serious problem, consider carefully
18 ALERT level C = Check. Ensure it is not caused by an omission or oversight
21 ALERT level G = General information/check it is not something unexpected

 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 ALERT type 2 Indicator that the structure model may be wrong or deficient
11 ALERT type 3 Indicator that the structure quality may be low
13 ALERT type 4 Improvement, methodology, query or suggestion
 0 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 22/03/2021; check.def file version of 19/03/2021

NOMOVE FORCED

Prob = 50
Temp = 293

59 Y

Z -140   K0705   P -1   R = 0.12   RES= O-144 X