checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: dg077_hy_dis01_compound_6f

Bond precision: C-C = 0.0058 A   Wavelength=0.71073

Cell: a=15.017(2)   b=8.913(1)   c=13.245(1)
                   alpha=90   beta=98.21(1)   gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	1754.6(3)	1754.6(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	?
Moiety formula	C13 H20 N2 P, C F3 O3 S	C13 H20 N2 P, C F3 O3 S
Sum formula	C14 H20 F3 N2 O3 P S	C14 H20 F3 N2 O3 P S
Mr	384.36	384.35
Dx,g cm-3	1.455	1.455
Z	4	4
Mu (mm-1)	0.321	0.321
F000	800.0	800.0
F000'	801.36	
h,k,lmax	17,10,15	17,10,15
Nref	3096	3086
Tmin,Tmax	0.962,0.984	
Tmin'	0.880	

Correction method= Not given

Data completeness= 0.997   Theta(max)= 25.020

R(reflections)= 0.0574(1896)   wR2(reflections)= 0.1433(3086)

S = 1.030   Npar= 217

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

PLAT222_ALERT_3_C Large Non-Solvent   H   Ueq(max)/Ueq(min) ...   3.09 Ratio
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ..   6
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of   S1
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of   C1

Alert level G

PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety   C16

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   0 ALERT level A = In general: serious problem
   0 ALERT level B = Potentially serious problem
   4 ALERT level C = Check and explain
   1 ALERT level G = General alerts; check

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 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
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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*, 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 13/08/2009; check.def file version of 12/08/2009