

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: s01

Bond precision: C-C = 0.0036 A Wavelength=0.71073

Cell: a=6.842(4) b=8.792(5) c=13.740(7)
 alpha=78.49(4) beta=85.24(2) gamma=84.24(2)

Temperature: 100 K

	Calculated	Reported
Volume	804.1(8)	804.2(7)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C11 H16 N2 P, C F3 O3 S	?
Sum formula	C12 H16 F3 N2 O3 P S	C12 H16 F3 N2 O3 P S
Mr	356.31	356.30
Dx,g cm-3	1.472	1.471
Z	2	2
Mu (mm-1)	0.344	0.343
F000	368.0	368.0
F000'	368.67	
h,k,lmax	8,10,16	8,10,16
Nref	3166	3160
Tmin,Tmax	0.872,0.934	
Tmin'	0.872	

Correction method= Not given

Data completeness= 0.998 Theta(max)= 26.000

R(reflections)= 0.0397(2311) wR2(reflections)= 0.1086(3160)

S = 0.961 Npar= 201

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

PLAT242_ALERT_2_C Check Low	Ueq as Compared to Neighbors for	S1
PLAT242_ALERT_2_C Check Low	Ueq as Compared to Neighbors for	C12
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor		2.15

0 ALERT level A = In general: serious problem

0 **ALERT level B** = Potentially serious problem
3 **ALERT level C** = Check and explain
0 **ALERT level G** = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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

