checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 7

Bond precision:	C-C = 0.0052 A	Wavelength=0.71073			
Cell:	a=10.2664(5) alpha=90	b=15.233 beta=90	8(8)	c=20.090 gamma=90	6(11)
Temperature:	173 K				
	Calculated		Reported	1	
Volume	3142.1(3)		3142.1(3	3)	
Space group	P 21 21 21		P2(1)2(1	L)2(
Hall group	P 2ac 2ab		?		
Moiety formula	C21 H13 B Cu F21	N7 03	?		
Sum formula	C21 H13 B Cu F21	N7 03	C21 H13	B Cu F21	N7 03
Mr	884.74		884.73		
Dx,g cm-3	1.870		1.870		
Z	4		4		
Mu (mm-1)	0.860		0.860		
F000	1740.0		1740.0		
F000'	1742.96				
h,k,lmax	13,20,26		13,20,26	5	
Nref	4341[7780]		7020		
Tmin,Tmax	0.814,0.918		0.725,0.	.919	
Tmin'	0.709				
Correction meth	od= MULTI-SCAN				
Data completene	ss= 1.62/0.90	Theta(ma	ax)= 28.2	240	
R(reflections)=	0.0436(6269)	wR2(ref]	lections)= 0.0968	(7020)
s = 1.084	Npar=	490			
The following ALER	IS were generated. Ea	ch ALERT has	the forma	ıt	
test-name_A Click on the hyper	LERT_alert-type_alert links for more detail	-level . s of the tes	t.		
Alert level A plat220_alert_2_a	Large Non-Solvent	F Ueq(ma	x)/Ueq(min	.)	4.90 Ratio
Alert level B	3 Check Low Ueq a	s Compared t	o Neighbor	rs for	C21

🏓 Alert level C		
PLAT213_ALERT_2_C Atom F19	has ADP max/min Ratio	3.20 prola
PLAT213_ALERT_2_C Atom F21	has ADP max/min Ratio	3.40 prola
PLAT220_ALERT_2_C Large Non	n-Solvent C Ueq(max)/Ueq(min)	3.06 Ratio
PLAT242_ALERT_2_C Check Low	v Ueq as Compared to Neighbors for	C20

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Alert level G
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
            correct. If it is not, please give the correct count in the
            _publ_section_exptl_refinement section of the submitted CIF.
           From the CIF: _diffrn_reflns_theta_max
From the CIF: _reflns_number_total
                                                               28.24
                                                               7020
           Count of symmetry unique reflns
                                                      4341
           Completeness (_total/calc)
                                                    161.71%
           TEST3: Check Friedels for noncentro structure
           Estimate of Friedel pairs measured
                                                     2679
           Fraction of Friedel pairs measured
                                                     0.617
           Are heavy atom types Z>Si present
                                                       yes
   1 ALERT level A = In general: serious problem
   1 ALERT level B = Potentially serious problem
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4 ALERT level C = Check and explain
1 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
6 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
1 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 12/11/2008; check.def file version of 12/11/2008

Datablock 7 - ellipsoid plot

