

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_n8cnb_0m_a

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: cu_n8cnb_0m_a

Bond precision: C-C = 0.0058 Å

Wavelength=1.54178

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Cell:      a=14.7541(12)
           alpha=66.335(5)
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b=16.6391 (12) c=17.6524 (14)
beta=80.415 (5) gamma=73.726 (5)

Temperature: 223 K

	Calculated	Reported
Volume	3802.9(5)	3802.9(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C84 H44 F24 N4 [+ solvent]	C84 H44 F24 N4
Sum formula	C84 H44 F24 N4 [+ solvent]	C84 H44 F24 N4
Mr	1565.23	1565.23
Dx, g cm-3	1.367	1.367
Z	2	2
Mu (mm-1)	1.064	1.064
F000	1584.0	1584.0
F000'	1590.57	
h, k, lmax	17, 20, 21	17, 20, 21
Nref	14047	13633
Tmin, Tmax	0.871, 0.890	0.653, 0.753
Tmin'	0.871	

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Correction method= # Reported T Limits: Tmin=0.653 Tmax=0.753
AbsCorr = MULTI-SCAN
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Data completeness= 0.971

$$\text{Theta (max)} = 68.642$$

R(reflections)= 0.0748(8775)

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wR2 (reflections)=  
0.1910 ( 13633)
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$$S = 1.037$$

Npar= 1199

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

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full value Low	0.975	Why?
PLAT213_ALERT_2_C	Atom C2A has ADP max/min Ratio	3.1	oblate
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.9	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.4	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C52 --C54	0.18	Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C23	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C52	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00583	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.838	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	338 Report
	8 0 0, 0 1 0, 8 1 0, 9 1 0, 3 2 0, 7 2 0,		
	8 2 0, 9 2 0, -16 3 0, 7 3 0, 8 3 0, 9 3 0,		
	7 4 0, 8 4 0, -15 5 0, 7 5 0, 8 5 0, 2 6 0,		
	7 6 0, 9 14 0, 9 16 0, 6 17 0, 7 17 0, 8 17 0,		
	9 17 0, 10 17 0, -9-17 1, -8-17 1, -7-17 1, -6-17 1,		
	-7-16 1, -10-12 1, -11-11 1, -7 -8 1, -5 -8 1, -2 -8 1,		
	-7 -6 1, -9 -5 1, -8 -5 1, -7 -5 1, -4 -5 1, 15 -5 1,		
	-13 -4 1, -8 -4 1, -7 -4 1, -6 -4 1, -8 -3 1, -7 -3 1,		
	-6 -3 1, -2 -3 1, 16 -3 1, -9 -2 1, -8 -2 1, -7 -2 1,		
	-6 -2 1, -5 -2 1, -2 -2 1, -17 -1 1, -9 -1 1, -8 -1 1,		
	-7 -1 1, -6 -1 1, -5 -1 1, -4 -1 1, -3 -1 1, -2 -1 1,		
	-8 0 1, -7 0 1, -6 0 1, -5 0 1, -4 0 1, -1 0 1,		
	-8 1 1, -7 1 1, -6 1 1, -5 1 1, 1 1 1, 9 1 1,		
	-16 2 1, 3 2 1, 16 2 1, -16 3 1, 0 3 1, 4 3 1,		
	9 3 1, -15 4 1, 1 4 1, 8 4 1, -15 5 1, 8 5 1,		
	8 6 1, 9 6 1, 14 6 1, 9 10 1, 15 11 1, 11 12 1,		

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	45	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms	40	Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.005	Degree
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	54	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	5	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	10	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0100	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for SecondPar	0.0200	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0100	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for SecondPar	0.0200	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0100	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for SecondPar	0.0200	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0100	Report
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PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0100	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for SecondPar	0.0200	Report

[illegible]

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PLAT434_ALERT_2_G Short Inter HL..HL Contact F8      ..F23      .      2.82 Ang.
                                     1-x,1-y,-z =      2_665 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure .....      ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....      9 Note
      H1AA      H1AB      H1AC      H2AA      H2AB      H2AC      H3AA      H3AB
      H3AC
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....      914 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed      ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      76 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File      1 Note
      1      1      1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....      2.7 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      2.66 Note
      Predicted wr2: Based on SigI**2 7.19 or SHELX Weight 19.28
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      0 Info

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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.

