

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) deh213

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: deh213

Bond precision:	C-C = 0.0048 A	Wavelength=0.71073
Cell:	a=27.3393(13)	b=25.0872(11) c=17.9939(9)
	alpha=90	beta=128.556(1) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	9651.0(8)	9651.0(8)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C54 H44 Cu N2 P2), 2(F6 P), C Cl2	?
Sum formula	C109 H88 Cl2 Cu2 F12 N4 P6	C109 H88 Cl2 Cu2 F12 N4 P6
Mr	2065.65	2065.63
Dx,g cm-3	1.422	1.422
Z	4	4
Mu (mm-1)	0.671	0.671
F000	4240.0	4240.0
F000'	4247.98	
h,k,lmax	43,39,28	43,39,28
Nref	20303	18551
Tmin,Tmax	0.851,0.941	0.664,0.747
Tmin'	0.807	

Correction method= # Reported T Limits: Tmin=0.664 Tmax=0.747

AbsCorr = MULTI-SCAN

Data completeness= 0.914 Theta(max)= 34.390

R(reflections)= 0.0580(11902) wR2(reflections)= 0.1706(18551)

S = 1.000 Npar= 645

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

PLAT230_ALERT_2_C	Hirshfeld Test Diff for C32	--C33	.	6.0 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference P3	--F3B		0.16 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C26	Check
PLAT336_ALERT_2_C	Long Bond Distance for C55	-Cl1		1.879 Ang.
PLAT336_ALERT_2_C	Long Bond Distance for C55_a	-Cl1		1.901 Ang.
PLAT411_ALERT_2_C	Short Inter H...H Contact H26	..H26		2.02 Ang.
		-x,y,1/2-z =	2_555	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.301	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).		8	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	5	Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers		1	Check



Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		19.20	Why ?
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group	C2/c	12/a	Note
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P4	--F5B	.	6.3 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P4	--F6A	.	6.7 s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		P4	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		P3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F5A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F5B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F6A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F6B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F3A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F3B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C55	Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		57%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		29%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)		33%	Note
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C28	Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		7	Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	1738	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		3	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		2	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
10 **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

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

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.

