

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cut83_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: cut83_a

Bond precision: C-C = 0.0047 Å Wavelength=0.71073

Cell: a=19.950 (4) b=20.310 (4) c=40.550 (8)
 alpha=91.68 (3) beta=99.57 (3) gamma=94.23 (3)
Temperature: 100 K

	Calculated	Reported
Volume	16143 (6)	16143 (6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	6(C90 H66 Cu2 N24 O3), 24(B C90 H66 Cu2 N24 O3, 4(B F4), 4.667(C4 H10 O), C4 O, F4), 5.5(C2 H3 N), 0.778(C4 H10 O), 0.1	
Sum formula	C628.67 H541.67 B24 Cu12 F96 N177 O24.67	C104.78 H90.28 B4 Cu2 F16 N29.50 O4.11
Mr	13816.80	2302.78
Dx, g cm ⁻³	1.421	1.421
Z	1	6
Mu (mm ⁻¹)	0.490	0.490
F000	7082.0	7082.0
F000'	7089.18	
h, k, lmax	24, 25, 50	24, 24, 50
Nref	63602	60876
Tmin, Tmax	0.889, 0.952	
Tmin'	0.822	

Correction method= Not given

Data completeness= 0.957

Theta(max)= 26.022

R(reflections)= 0.0601(51462)

wR2(reflections)=
0.1838(60876)

S = 1.021

Npar= 4527

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 B

PLAT201_ALERT_2_B	Isotropic non-H Atoms in Main Residue(s)	6 Report
N1F	C1F C2F C3F C4F	etc.

Author Response: Orientational disorder was present in one helicate (ligand F at the Cu3 end). The low electron density associated with the second part prevented its modelling, and this residual electron density caused problems in modelling the main part anisotropically.

Alert level C

PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	8 Check
	O1ET C2ET C3ET C1ET C4ET N1T2	etc.
PLAT220_ALERT_2_C	NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range	3.3 Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C5F Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C12F Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C3EU Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C1S1 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C1T6 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C1T1 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C1S2 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C1T9 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C1T4 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C1S3 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C1S6 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C1T2 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including O1EU	0.109 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including F17B	0.136 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including F45B	0.129 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including N1T9	0.114 Check
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4	Please Check
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1 Note
	C90 H66 Cu2 N24 O3	
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	1090 Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	22 Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.71Ang From C1T8	1.80 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.04Ang From N1T7 .	1.45 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.94Ang From N1T8 .	0.84 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H4F .	-0.43 eA-3

Alert level G

[illegible]

[illegible]

PLAT300_ALERT_4_G	Atom Site Occupancy of H2TR	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1T7	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1T7	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2T7	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2TY	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Hb	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Hc	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1W	Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 7)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 8)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 9)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 11)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 15)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 16)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 18)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 19)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 20)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 21)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 22)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 23)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 24)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 40)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 41)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 42)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 43)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 44)		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 7)		3.40	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 8)		2.55	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 11)		2.75	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 15)		3.31	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 19)		2.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 20)		1.60	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 22)		2.45	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 23)		2.25	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 24)		1.69	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 44)		0.50	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		O1W	Check
PLAT315_ALERT_2_G	Singly Bonded Carbon Detected (H-atoms Missing).		C1EV	Check
PLAT315_ALERT_2_G	Singly Bonded Carbon Detected (H-atoms Missing).		C4EV	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H7A ..Hc .		2.11	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F14A ..C24B .		2.89	Ang.
		1+x,y,z =	1_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F18A ..C7F .		2.96	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F19A ..C2T8 .		2.91	Ang.
		x,1+y,z =	1_565	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C27C ..C2T3 .		3.19	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C28C ..C2T3 .		3.17	Ang.
		x,y,z =	1_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		157	Note
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		5	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	C90 H66 Cu2 N24 O3			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		3	Note
	C90 H66 Cu2 N24 O3			

PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	4 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	5 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	6 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	7 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	8 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	9 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	10 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	11 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	12 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	13 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	14 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	15 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C4 H10 O	16 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C4 H10 O	17 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C4 H10 O	18 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C4 O	19 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	20 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	21 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	22 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	23 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # B F4	24 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C2 H3 N	25 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C2 H3 N	26 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C2 H3 N	27 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C2 H3 N	28 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C2 H3 N	29 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C2 H3 N	30 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C2 H3 N	31 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	32 Note

C2 H3 N			
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		33	Note
C2 H3 N			
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		34	Note
C2 H3 N			
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		35	Note
C2 H3 N			
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		36	Note
C2 H3 N			
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		37	Note
C2 H3 N			
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		38	Note
C2 H3 N			
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		39	Note
C2 H3 N			
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		40	Note
C2 H3 N			
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		41	Note
C2 H3 N			
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		42	Note
C2 H3 N			
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		43	Note
C2 H3 N			
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		44	Note
O			
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (I) .	1.16	Info	
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2 (I) .	1.20	Info	
PLAT794_ALERT_5_G Tentative Bond Valency for Cu3 (II) .	2.13	Info	
PLAT794_ALERT_5_G Tentative Bond Valency for Cu4 (I) .	1.22	Info	
PLAT794_ALERT_5_G Tentative Bond Valency for Cu5 (I) .	1.16	Info	
PLAT794_ALERT_5_G Tentative Bond Valency for Cu6 (I) .	1.16	Info	
PLAT860_ALERT_3_G Number of Least-Squares Restraints	774	Note	
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .		Please Do !	
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).	1	Note	
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	1621	Note	
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF	3	Note	
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	9	Note	
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	1	Info	

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 27 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 213 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 26 ALERT type 2 Indicator that the structure model may be wrong or deficient
 44 ALERT type 3 Indicator that the structure quality may be low
 161 ALERT type 4 Improvement, methodology, query or suggestion
 6 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.

