



## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UPC-114

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: UPC-114

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Bond precision:	C-C = 0.0072 Å	Wavelength=0.71073	
Cell:	a=40.980 (6) alpha=90	b=40.980 (6) beta=90	c=57.955 (12) gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	97327 (35)	97328 (34)	
Space group	I 4/m m m	I 4/m m m	
Hall group	-I 4 2	-I 4 2	
Moiety formula	C337 H214 Cu24 N12 O114 [+ solvent]	?	
Sum formula	C337 H214 Cu24 N12 O114 [+ solvent]	C337 H214 Cu24 N12 O114	
Mr	7780.41	7780.15	
Dx, g cm <sup>-3</sup>	0.531	0.530	
Z	4	4	
Mu (mm <sup>-1</sup> )	0.544	0.544	
F000	15712.0	15656.0	
F000'	15749.81		
h, k, lmax	47, 47, 67	47, 47, 67	
Nref	21360	21286	
Tmin, Tmax	0.849, 0.887	0.854, 0.890	
Tmin'	0.849		



PLAT241_ALERT_2_C	High	MainResAtom	Ueq as Compared to Neighbours	C25	Check
PLAT241_ALERT_2_C	High	MainResAtom	Ueq as Compared to Neighbours	C28	Check
PLAT241_ALERT_2_C	High	MainResAtom	Ueq as Compared to Neighbours	C36	Check
PLAT241_ALERT_2_C	High	MainResAtom	Ueq as Compared to Neighbours	C39	Check
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	Cu2	Check
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	Cu3	Check
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	Cu4	Check
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	Cu6	Check
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	Cu7	Check
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	C12	Check
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	C18	Check
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	C26	Check
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	C27	Check
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	C33	Check
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	C37	Check
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	C40	Check
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	C44	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	Cu1	0.158	Check
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)	.....		017	Check
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist.	C10 -C15	.	1.37	Ang.
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	.....		0.00716	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond	C9 - C10	.	1.53	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond	C20 - C27	.	1.53	Ang.
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N1 --H1A	.	Please	Check

**Author Response: Isolated coordinated water molecule without H bond acceptor.**

PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N1 --H1B	.	Please	Check
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**Author Response: Isolated coordinated water molecule without H bond acceptor.**

PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N2 --H2A	.	Please	Check
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**Author Response: Isolated coordinated water molecule without H bond acceptor.**

PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N2 --H2B	.	Please	Check
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**Author Response: Isolated coordinated water molecule without H bond acceptor.**

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....		4.311	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.581		89	Report
	1 1 0, 0 2 0, 2 2 0, 4 4 0, 6 6 0, 0 10 0,				
	12 12 0, 15 15 0, 19 21 0, 3 6 1, 7 14 1, 12 33 1,				
	0 0 2, 0 2 2, 4 6 2, 11 25 2, 6 36 2, 0 5 3,				
	1 6 3, 2 2 4, 3 3 4, 2 6 4, 3 12 5, 17 19 6,				
	3 21 6, 10 24 6, 0 0 8, 9 9 8, 5 21 8, 3 29 8,				
	( 59 More NOT listed: see .ckf listing file)				

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**Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	22	Note
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PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H-Atoms	30	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	12	Report
	H1A H1B H2A H2B H13 H14 H15 H16		
	H18 H17 H19A H19B		
PLAT014_ALERT_1_G	N.O.K. _shelx_fab_checksum Found in CIF .....	Please	Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGH T Unusually Large	196.96	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	2	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	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	0.0150	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT299_ALERT_4_G	Atom Site Occupancy Constrained at .....	0.5	Check
	H2A H2B H15 H16 H18		
PLAT299_ALERT_4_G	Atom Site Occupancy Constrained at .....	0.25	Check
	O19 C45 H17 H19A H19B H45		
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1)	1%	Note
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C10 -C15	0.15	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact N2 ..C38 .	2.98	Ang.
	1/2+y, 1/2-x, 1/2-z =	26_555	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Crystal Structure	!	Info
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	7.60	Deg.
	C45 -O17 -C45 1_555 1_555 4_655 .....	# 158	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	7.60	Deg.
	C45 -O17 -C45 20_555 1_555 17_655 .....	# 161	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	28.80	Deg.
	C45 -O17 -H17 20_555 1_555 1_555 .....	# 168	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	28.80	Deg.
	C45 -O17 -H17 17_655 1_555 1_555 .....	# 170	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	28.80	Deg.
	C45 -O17 -H17 1_555 1_555 3_555 .....	# 172	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	28.80	Deg.
	C45 -O17 -H17 4_655 1_555 3_555 .....	# 174	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	23.90	Deg.
	O17 -C45 -H17 17_655 1_555 17_655 .....	# 337	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	23.90	Deg.
	O17 -C45 -H17 1_555 1_555 3_555 .....	# 340	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	25.10	Deg.
	H45 -C45 -H45 1_555 1_555 4_655 .....	# 347	Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	3	Check
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers	1	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	444	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please	Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	35%	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	50	Note
	4 9 9, 6 7 9, 5 21 8, 3 29 8, 6 13 27, 6 7 19,		
	5 8 9, 3 18 13, 4 13 13, 1 1 0, 9 9 12, 9 27 12,		
	7 7 16, 11 13 16, 2 6 4, 6 6 22, 4 6 2, 2 2 0,		
	3 6 1, 2 11 11, 6 7 29, 6 36 2, 12 33 1, 10 24 6,		
	9 12 21, 5 18 15, 2 13 23, 3 12 5, 1 13 12, 7 20 23,		
	11 20 19, 8 18 10, 16 16 12, 0 0 2, 6 11 17, 2 9 9,		

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4 26 12, 14 14 16, 3 21 6, 11 14 23, 2 2 4, 18 25 13,  
1 6 3, 17 19 6, 11 25 2, 7 14 1, 19 21 0, 6 7 21,  
4 14 22, 7 9 14,  
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... Please Check  
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check  
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree  
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 6.459 Note  
Predicted wR2: Based on SigI**2 4.18 or SHELX Weight 24.70  
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info  
PLAT994_ALERT_1_G SHELXL .ins Contains no or MERG 0 Instruction .. ! Note
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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
5 **ALERT level B** = A potentially serious problem, consider carefully  
37 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
44 **ALERT level G** = General information/check it is not something unexpected

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

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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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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**PLATON version of 15/01/2026; check.def file version of 02/01/2026**

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## **duplicate check**

**No duplication found**

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