

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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_20230904_XAJT_28_S_1_0m_sq

Bond precision:	C-C = 0.0402 Å	Wavelength=1.54178	
Cell:	a=59.444 (6) alpha=90	b=59.444 (6) beta=90	c=167.23 (3) gamma=120
Temperature:	150 K		
	Calculated	Reported	
Volume	511754 (138)	511754 (140)	
Space group	R -3	R -3 :H	
Hall group	-R 3	-R 3	
Moiety formula	C744 N28 O48 P48 Pt24 [+ solvent]	?	
Sum formula	C744 N28 O48 P48 Pt24 [+ solvent]	C744 N28 O48 P48 Pt24	
Mr	16264.26	16264.44	
Dx, g cm ⁻³	0.633	0.633	
Z	12	12	
Mu (mm ⁻¹)	4.207	4.207	
F000	91632.0	91632.0	
F000'	90687.55		
h, k, lmax	59, 59, 167	55, 58, 167	
Nref	120311	114995	
Tmin, Tmax	0.634, 0.657	0.432, 0.750	
Tmin'	0.507		

Correction method= # Reported T Limits: Tmin=0.432 Tmax=0.750

AbsCorr = MULTII-SCAN

Data completeness= 0.956

Theta(max)= 50.667

R(reflections)= 0.1570(25210)

wR2(reflections)=
0.3856(114995)

S = 1.608

Npar= 4896

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 A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550

Calculated sin(theta_max)/wavelength = 0.5017

Author Response: Crystal diffracted very weakly, but it is already the best resolution.

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18

Rint given 0.233

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12	0.233	Report
PLAT029_ALERT_3_B _diffn_measured_fraction_theta_full value Low .	0.956	Why?
PLAT082_ALERT_2_B High R1 Value	0.16	Report
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25)	0.39	Report
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of	Pt16	Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of	P1_38	Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of	C1_36	Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of	Pt13	Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of	Pt15	Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of	N1_10	Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of	C3_31	Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including	Pt3	0.309 Check
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds	0.04021	Ang.

Alert level C

PLAT213_ALERT_2_C Atom O5_9	has ADP max/min Ratio	3.8	prolat
PLAT213_ALERT_2_C Atom C6_43	has ADP max/min Ratio	3.5	prolat
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt1	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt2	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt3	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt4	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt5	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt6	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt7	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt8	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt9	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt10	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt11	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt12	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt13	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt14	.	6	Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Pt15	.	6	Check

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[illegible]

[illegible]

[illegible]

[illegible]

PLAT218_ALERT_3_C	Constrained U(ij)	Components(s) for C490#	.	6	Check
PLAT218_ALERT_3_C	Constrained U(ij)	Components(s) for P31#	.	6	Check
PLAT218_ALERT_3_C	Constrained U(ij)	Components(s) for C491#	.	6	Check
PLAT218_ALERT_3_C	Constrained U(ij)	Components(s) for C492#	.	6	Check
PLAT218_ALERT_3_C	Constrained U(ij)	Components(s) for C493#	.	6	Check
PLAT218_ALERT_3_C	Constrained U(ij)	Components(s) for C494#	.	6	Check
PLAT218_ALERT_3_C	Constrained U(ij)	Components(s) for C495#	.	6	Check
PLAT218_ALERT_3_C	Constrained U(ij)	Components(s) for C496#	.	6	Check
PLAT218_ALERT_3_C	Constrained U(ij)	Components(s) for P32#	.	6	Check
PLAT220_ALERT_2_C	NonSolvent	Resd 1 C Ueq(max)/Ueq(min) Range		3.7	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 2 C Ueq(max)/Ueq(min) Range		5.8	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 2 P Ueq(max)/Ueq(min) Range		3.6	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 2 Pt Ueq(max)/Ueq(min) Range		3.1	Ratio
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	P1_14		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	P1_19		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C5_1		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C15_1		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C23_1		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C32_3		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C35_3		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C38_3		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C42_3		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C46_3		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C58_3		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C61_3		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C63_3		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C65_3		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C67_3		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C68_3		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C13_5		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C8_6		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C12_6		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C15_6		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C21_6		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C1_17		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C5_17		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C1_27		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	P1_36		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	P1_39		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	P1_41		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	P1_42		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	N1_9		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C1_10		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C8_10		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C25_10		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C56_10		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C58_10		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C61_10		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C63_10		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C71_10		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C10_8		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C14_8		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C3_9		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C10_11		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C16_11		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C24_11		Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C1_34		Check

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PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C34_9	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C38_9	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C41_9	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C5_11	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C11_11	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C5_28	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C1_31	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C5_32	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C5_33	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C1_38	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C3_38	Check
PLAT260_ALERT_2_C	Large Average	Ueq of Residue Including	Pt1	0.216	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen	(C-O > 1.3 Ang)		O3_1	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen	(C-O > 1.3 Ang)		O7_1	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen	(C-O > 1.3 Ang)		O4_5	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen	(C-O > 1.3 Ang)		O4_8	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen	(C-O > 1.3 Ang)		O3_9	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen	(C-O > 1.3 Ang)		O7_9	Check



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	582	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	588	Report
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..		Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	1020.00	Why ?
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	-2	Units
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	9	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	1	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	11	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	11	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	4	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0100	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0100	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0100	Report
PLAT432_ALERT_2_G	Short Inter X...Y Contact O10_9 ..C6_19 .	3.02	Ang.
	x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C4_20 ..C4_33 .	2.24	Ang.
	1-x,1-y,1-z =	10_666	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C2_23 ..C6_38 .	3.16	Ang.
	1-x+y,1-x,z =	3_665	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	!	Info
PLAT608_ALERT_4_G	ADDSYM Test Skipped (Too Time-consuming)	!	Info
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	580	Note
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C33_9 --C6_40	1.76	Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	20773	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	88	Note
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	4	Units

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

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

