

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: 1

Bond precision:	C-C = 0.0035 A	Wavelength=0.71073
Cell:	a=27.5082(16)	b=9.2312(5) c=20.6915(12)
	alpha=90	beta=92.558(2) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	5249.0(5)	5249.0(5)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	?
Moiety formula	C24 H30 Cu F2 N4 O5, 2(H2 O)	?
Sum formula	C24 H34 Cu F2 N4 O7	C24 H34 Cu F2 N4 O7
Mr	592.10	592.10
Dx, g cm-3	1.498	1.498
Z	8	8
Mu (mm-1)	0.897	0.897
F000	2472.0	2472.0
F000'	2475.78	
h, k, lmax	35, 12, 26	35, 12, 26
Nref	12099	12040
Tmin, Tmax	0.493, 0.639	0.910, 0.982
Tmin'	0.483	

Correction method= # Reported T Limits: Tmin=0.910 Tmax=0.982
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 27.550

R(reflections)= 0.0426(8696) wR2(reflections)= 0.1050(12040)

S = 1.023 Npar= 675

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

PLAT165_ALERT_3_C	Nr. of Status R Flagged Non-Hydrogen Atoms	4
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	C2 Check
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	C26 Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D H6W2 .. H1W1 ..	2.14 Ang.

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	18 Note
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	12 Report
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	0.80 mm
PLAT093_ALERT_1_G	No su's on H-positions, refinement reported as .	mixed Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293 Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu2 -- N2 ..	6.8 su
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	12 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II)	2.15 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu2 (II)	2.17 Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	18 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note

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

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

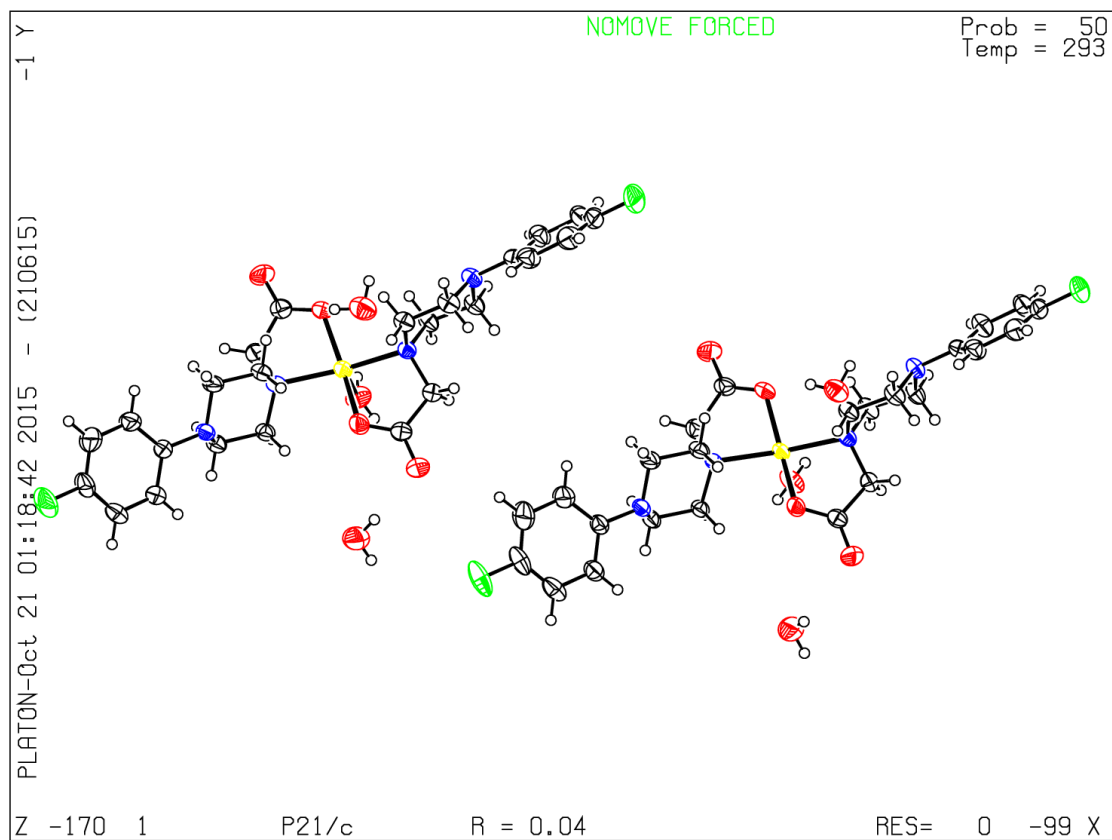
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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*, 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.



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Datablock: 1

Bond precision: C-C = 0.0062 Å

Wavelength=0.71073

Cell: a=6.6508(6) b=7.2655(6) c=15.3900(14)
 alpha=95.281(3) beta=95.647(3) gamma=115.921(2)
Temperature: 293 K

	Calculated	Reported
Volume	657.99(10)	657.98(10)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C24 H32 F2 N4 Ni O6	?
Sum formula	C24 H32 F2 N4 Ni O6	C24 H32 F2 N4 Ni O6
Mr	569.23	569.23
Dx, g cm-3	1.436	1.437
Z	1	1
Mu (mm-1)	0.797	0.797
F000	298.0	298.0
F000'	298.48	
h, k, lmax	8, 8, 18	8, 8, 18
Nref	2440	2413
Tmin, Tmax	0.569, 0.727	0.789, 0.820
Tmin'	0.523	

Correction method= # Reported T Limits: Tmin=0.789 Tmax=0.820
AbsCorr = MULTI-SCAN

Data completeness= 0.989

Theta(max)= 25.490

R(reflections)= 0.0374(2264)

wR2(reflections)= 0.0980(2413)

S = 1.095

Npar= 166

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test-name_ALERT_alert-type_alert-level.

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● Alert level C

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
aquamarine
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.65 Report
PLAT165_ALERT_3_C Nr. of Status R Flagged Non-Hydrogen Atoms 1
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for C9 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C10 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.5 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.0062 Ang.

● Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size 0.80 mm
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as . mixed Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 1 Do !
O2 -NI1 -O2 -C1 -48.00 78.00 2.656 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 10 Do !
N2 -NI1 -N2 -C2 18.00 0.00 2.656 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 15 Do !
N2 -NI1 -N2 -C3 7.00 0.00 2.656 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 20 Do !
N2 -NI1 -N2 -C6 6.00 0.00 2.656 1.555 1.555 1.555
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 2 Note
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PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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