

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: ic11831

Bond precision: C-C = 0.0130 A Wavelength=0.71073

Cell: a=16.9785(9) b=22.6333(12) c=13.0677(7)
alpha=90 beta=90.791(1) gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	5021.2(5)	5021.2(5)
Space group	C 2/m	C2/m
Hall group	-C 2y	?
Moiety formula	C88 H72 N16 Ni4 O8, F6 P, 4(C2 H3 Cl3)	?
Sum formula	C96 H84 Cl12 F6 N16 Ni4 O8 P	C96 H84 Cl12 F6 N16 Ni4 O8 P
Mr	2394.92	2395.00
Dx,g cm-3	1.584	1.584
Z	2	2
Mu (mm-1)	1.150	1.150
F000	2442.0	2442.0
F000'	2449.28	
h,k,lmax	22,29,16	22,29,16
Nref	5912	5910
Tmin,Tmax	0.715,0.795	0.724,0.803
Tmin'	0.701	

Correction method= MULTI-SCAN

Data completeness= 1.000 Theta(max)= 27.500

R(reflections)= 0.0902(3965) wR2(reflections)= 0.2622(5910)

S = 1.037 Npar= 290

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)

● Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
Weighted R factor given 0.262

PLAT084_ALERT_2_C High wR2 Value 0.26
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.01
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 1
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for N3
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of P1
PLAT303_ALERT_2_C Full Occupancy H-Atom H21A with # Connections 2
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 13
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C45 - C46 ... 1.35 Ang.
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond C33 - C34 ... 1.38 Ang.

● Alert level G

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.13
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 31.93
PLAT242_ALERT_2_G Check Low Ueq as Compared to Neighbors for C2
PLAT301_ALERT_3_G Note: Main Residue Disorder 86 Perc.
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder 33 Perc.
PLAT432_ALERT_2_G Short Inter X...Y Contact C12 .. C13 .. 3.12 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C12 .. C14 .. 3.15 Ang.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 2.50 Ratio
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C3 -- C41 . 1.76 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C3 -- C42 . 1.90 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C5 -- C39 . 1.72 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C8 -- C9 . 1.72 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C9 -- C8 . 1.72 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C14 -- C15 . 1.85 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C15 -- C14 . 1.85 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C21 -- C21 . 1.74 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C30 -- C36 . 1.83 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C36 -- C30 . 1.83 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C39 -- C5 . 1.72 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C41 -- C3 . 1.76 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C42 -- C3 . 1.90 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 69
C8 -N1 -C8 1.555 1.555 6.555 30.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 82
C8 -N2 -C8 1.555 1.555 6.555 34.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 88
C15 -N3 -C15 1.555 1.555 6.555 44.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 98
C15 -N4 -C15 1.555 1.555 6.555 37.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 114
C30 -N5 -C37 1.555 1.555 2.555 32.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 126
C30 -N6 -C37 1.555 1.555 2.555 37.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 137
C37 -N7 -C30 1.555 1.555 2.555 39.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 146
C37 -N8 -C30 1.555 1.555 2.555 35.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 159
O1 -C1 -O4 1.555 1.555 5.555 19.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 167
C40 -C2 -C7 5.555 1.555 1.555 20.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 172

	01	-C2	-04	1.555	1.555	5.555		19.90	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C2	-C3	-C41	1.555	1.555	5.555		14.00	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C41	-C3	-C42	5.555	1.555	5.555		43.20	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C6	-C5	-C39	1.555	1.555	5.555		5.30	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C39	-C6	-C7	5.555	1.555	1.555		38.00	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C7	-C6	-C40	1.555	1.555	5.555		19.20	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C41	-C7	-C2	5.555	1.555	1.555		22.00	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C39	-C7	-C6	5.555	1.555	1.555		11.70	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	N1	-C8	-N1	1.555	1.555	6.555		40.60	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C9	-C8	-C9	1.555	1.555	6.555		37.30	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C10	-C9	-C10	1.555	1.555	6.555		21.20	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C8	-C9	-C8	1.555	1.555	6.555		28.70	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C9	-C10	-C9	1.555	1.555	6.555		41.80	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C10	-C11	-C10	1.555	1.555	6.555		23.10	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C13	-C11	-C13	1.555	1.555	6.555		29.40	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C13	-C14	-C13	1.555	1.555	6.555		25.60	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C15	-C14	-C15	1.555	1.555	6.555		36.10	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C14	-C15	-C14	1.555	1.555	6.555		44.50	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C26	-C16	-C17	2.555	1.555	1.555		10.20	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C18	-C17	-C25	1.555	1.555	2.555		28.30	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C26	-C17	-C16	2.555	1.555	1.555		40.00	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C24	-C18	-C19	2.555	1.555	1.555		16.40	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C17	-C18	-C26	1.555	1.555	2.555		12.20	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C25	-C19	-C18	2.555	1.555	1.555		27.80	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	O3	-C19	-O2	2.555	1.555	1.555		26.20	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C19	-C20	-C24	1.555	1.555	2.555		14.10	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	O2	-C22	-O3	1.555	1.555	2.555		25.20	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	O3	-C23	-O2	1.555	1.555	2.555		26.70	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	O2	-C24	-O3	2.555	1.555	1.555		27.80	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C18	-C24	-C25	2.555	1.555	1.555		27.20	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#
	C17	-C25	-C26	2.555	1.555	1.555		14.00	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF	#

	C19	-C25	-C24	2.555	1.555	1.555	15.70	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 401
	C25	-C26	-C18	1.555	1.555	2.555	26.50	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 406
	C17	-C27	-C26	2.555	1.555	1.555	14.10	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 418
	C24	-C29	-C19	1.555	1.555	2.555	14.00	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 429
	N6	-C30	-N7	1.555	1.555	2.555	15.80	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 439
	C31	-C30	-C36	1.555	1.555	2.555	34.40	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 446
	C32	-C31	-C35	1.555	1.555	2.555	20.10	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 450
	C30	-C31	-C37	1.555	1.555	2.555	35.80	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 456
	C31	-C32	-C36	1.555	1.555	2.555	42.30	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 462
	C32	-C33	-C35	2.555	1.555	1.555	22.70	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 466
	C32	-C33	-C35	1.555	1.555	2.555	22.70	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 471
	N7	-C34	-N6	1.555	1.555	2.555	16.20	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 475
	N7	-C34	-N6	2.555	1.555	1.555	16.20	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 482
	C36	-C35	-C31	1.555	1.555	2.555	40.30	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 488
	C35	-C36	-C32	1.555	1.555	2.555	22.10	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 492
	C37	-C36	-C30	1.555	1.555	2.555	31.20	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 502
	N7	-C37	-N6	1.555	1.555	2.555	13.50	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 507
	C36	-C37	-C31	1.555	1.555	2.555	39.00	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 510
	N8	-C37	-N5	1.555	1.555	2.555	44.00	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 515
	C6	-C38	-C39	5.555	1.555	1.555	16.50	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 529
	C7	-C39	-C40	5.555	1.555	1.555	21.40	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 531
	C6	-C39	-C5	5.555	1.555	5.555	19.00	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 537
	C2	-C40	-C41	5.555	1.555	1.555	23.10	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 544
	C39	-C40	-C6	1.555	1.555	5.555	13.00	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 554
	C40	-C41	-C7	1.555	1.555	5.555	21.90	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 556
	O4	-C41	-O1	1.555	1.555	5.555	20.80	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 560
	C2	-C41	-C3	5.555	1.555	5.555	39.00	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 567
	C41	-C42	-C2	1.555	1.555	5.555	17.60	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 577
	O1	-C44	-O4	5.555	1.555	1.555	17.50	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 583
	C2	-O1	-C41	1.555	1.555	5.555	22.20	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 585
	C44	-O1	-C1	5.555	1.555	1.555	22.30	Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in	CIF # 593

	C23	-O2	-C22	2.555	1.555	1.555	19.50 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in CIF #	595
	C24	-O2	-C19	2.555	1.555	1.555	15.40 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in CIF #	603
	C19	-O3	-C24	2.555	1.555	1.555	17.00 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in CIF #	605
	C23	-O3	-C22	1.555	1.555	2.555	18.00 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in CIF #	612
	C41	-O4	-C2	1.555	1.555	5.555	21.30 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in CIF #	616
	C1	-O4	-C44	5.555	1.555	1.555	20.00 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in CIF #	637
	F2	-P1	-F3	1.555	1.555	6.555	40.50 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in CIF #	643
	F2	-P1	-F3	1.555	1.555	5.456	40.50 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in CIF #	651
	F2	-P1	-F3	5.456	1.555	1.555	40.50 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle	in CIF #	659
	F2	-P1	-F3	5.456	1.555	2.456	40.50 Deg.
PLAT790_ALERT_4_G	Centre of Gravity not	Within	Unit Cell: Resd.	#			2
	F6	P					
PLAT790_ALERT_4_G	Centre of Gravity not	Within	Unit Cell: Resd.	#			3
	C2	H3	C13				
PLAT811_ALERT_5_G	No ADDSYM Analysis:	Too Many Excluded	Atoms				!

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 25 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 ALERT type 3 Indicator that the structure quality may be low
 87 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*, 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.

