

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sni1_0m

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: sni1_0m

Bond precision: C-C = 0.0064 A

Wavelength=0.71073

Cell: a=8.1911(2) b=11.6624(3) c=16.5356(4)
 alpha=108.812(1) beta=91.201(1) gamma=91.150(1)
Temperature: 295 K

	Calculated	Reported
Volume	1494.30(6)	1494.30(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C27 H27 N4 Ni O3, 2(N O3)	?
Sum formula	C27 H27 N6 Ni O9	C27 H27 N6 Ni O9
Mr	638.24	638.26
Dx,g cm-3	1.418	1.419
Z	2	2
Mu (mm-1)	0.710	0.710
F000	662.0	662.0
F000'	662.98	
h,k,lmax	10,15,22	10,15,22
Nref	7428	7409
Tmin,Tmax	0.837,0.899	0.812,0.901
Tmin'	0.837	

Correction method= # Reported T Limits: Tmin=0.812 Tmax=0.901
AbsCorr = MULTI-SCAN

Data completeness= 0.997

Theta(max)= 28.290

R(reflections)= 0.0679(5484)

wR2(reflections)= 0.2336(7409)

S = 1.099

Npar= 390

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

PLAT430_ALERT_2_A	Short Inter D...A Contact	O8	..	O9	..	0.84	Ang.
PLAT430_ALERT_2_A	Short Inter D...A Contact	O8	..	O8	..	1.97	Ang.
PLAT430_ALERT_2_A	Short Inter D...A Contact	O9	..	O9	..	2.45	Ang.

These were raised by the disorder oxygen atoms on nitrate anion

Alert level B

PLAT420_ALERT_2_B	D-H Without Acceptor	O2	-	H2D	..	Please	Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O7	..	O8	..	2.80	Ang.
PLAT934_ALERT_3_B	Number of (Iobs-Icalc)/SigmaW > 10 Outliers				3	Check

Alert level C

PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent				1	
PLAT220_ALERT_2_C	Large Non-Solvent C	Ueq(max)/Ueq(min) Range				3.4	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C19	--	C20	..	5.7	su
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C6	--	C7	..	0.18	Ang.
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for			C7	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for			C8	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for			C19	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for			C4	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of				N7	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of				N5	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds				0.0064	Ang.
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600				7	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much smaller I(calc)	.				1	Check
PLAT975_ALERT_2_C	Check Calcd Residual Density	0.56A From		O11		0.79	eA-3
PLAT976_ALERT_2_C	Check Calcd Residual Density	1.00A From		O2		-0.51	eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite					7	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				6	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.					0.14	Report
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal				0.00100	Degree
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	O1	--	C1	..	20.3	su
PLAT300_ALERT_4_G	Atom Site Occupancy of >O1	is Constrained at				0.650	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <O1'	is Constrained at				0.350	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *O10	is Constrained at				0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *O11	is Constrained at				0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *O12	is Constrained at				0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *O10_a	is Constrained at				0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *O11_a	is Constrained at				0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *O12_a	is Constrained at				0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *O7	is Constrained at				0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *O8	is Constrained at				0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *O9	is Constrained at				0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *N6	is Constrained at				0.500	Check
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage =			3	Note
PLAT302_ALERT_4_G	Anion/Solvent Disorder	Percentage =			50	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O8	..	N6	..	1.64	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O9	..	N6	..	1.93	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	N6	..	N6	..	2.13	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels				1	Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	.				1.27	Ratio
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				81	Check
	O9 -N6 -O8	1.555	1.555	2.777		29.90	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				89	Check
	O12 -N7 -O10	2.876	1.555	1.555		44.10	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				90	Check

	012	-N7	-O10	1.555	1.555	2.876		44.10	Deg.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #							2	Note
	N 03								
PLAT860_ALERT_3_G	Number of Least-Squares Restraints							5	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL							2014	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600							10	Note

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

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

PLATON version of 29/01/2015; check.def file version of 29/01/2015

