checkCIF/PLATON report

Structure factors have been supplied for datablock(s) T7_0ma

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: T7_0ma

Bond precision: C-C = 0.0080 A Wavelength=1.54178

Cell: a=21.1388(13) b=16.1802(10) c=21.3131(13)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	7289.7(8)	7289.7(8)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C26 H28 Br4 N4 Ni O2, 2(C2 H6 O S)	C26 H28 Br4 N4 Ni O2, 2(C2 H6 O S)
Sum formula	C30 H40 Br4 N4 Ni O4 S2	C30 H40 Br4 N4 Ni O4 S2
Mr	963.07	963.13
Dx,g cm-3	1.755	1.755
Z	8	8
Mu (mm-1)	7.301	7.301
F000	3840.0	3840.0
F000'	3806.30	
h,k,lmax	26,20,26	26,20,26
Nref	7211	6925
Tmin,Tmax	0.559,0.852	0.559,0.852
Tmin'	0.456	

Correction method= # Reported T Limits: Tmin=0.559 Tmax=0.852
AbsCorr = MULTI-SCAN

Data completeness= 0.960 Theta(max)= 72.471

R(reflections)= 0.0999(6753) wR2(reflections)= 0.3031(6925)

S = 1.456 Npar= 411

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

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.90Ang From Br4 3.01 eA-3

Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.01Ang From Br3 2.99 eA-3

Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.08Ang From Br1 2.89 eA-3

Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.07Ang From Br2 2.88 eA-3

Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.05Ang From Br4 2.87 eA-3

Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.88Ang From Br1 2.86 eA-3

Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.90Ang From Br2 2.69 eA-3

Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.71Ang From Br1 -2.51 eA-3

Author Response: This might be caused by wrongly assigned atom types and other model errors. But It was also confirmed from (1H)NMR and HRMS that our crystal structure is correct.It has been tried with various models considering different type of solvent molecules. But DMSO (which was used as solvent for crystallization) shows the most acceptable model.

Alert level C

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DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.30 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       3.13 eA-3
PLAT324_ALERT_2_C Check for Possibly Missing H on Coordinating....         N2 Check
PLAT324_ALERT_2_C Check for Possibly Missing H on Coordinating....        N18 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............      0.008 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H19A     ..H40C     .       2.14 Ang.
                                                    x,y,z  =      1_555 Check
PLAT431_ALERT_2_C Short Inter HL..A Contact  Br1      ..S38      .       3.50 Ang.
                                       1/2-x,1-y,-1/2+z  =      4_564 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.461 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        132 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.82Ang From Br3             2.48 eA-3
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Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.02Ang From Br1             1.97 eA-3
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Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.17Ang From Br2             1.88 eA-3
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Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.95Ang From Ni1             1.76 eA-3
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Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.99Ang From N18             1.71 eA-3
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Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.21Ang From Br3   1.70 eA-3

Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.29Ang From C13   1.64 eA-3

Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.22Ang From Br4   1.57 eA-3

Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.22Ang From Br4   1.56 eA-3

Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.33Ang From C32   1.54 eA-3

Author Response: It is because of repealed electrons of heavy elements like bromine (Br1, Br2, Br3 and Br4) atom which is not unusual.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.81Ang From Br4   -2.37 eA-3

Author Response: This might be caused by wrongly assigned atom types and other model errors. But It was also confirmed from (1H)NMR and HRMS that our crystal structure is correct.It has been tried with various models considering different type of solvent molecules. But DMSO (which was used as solvent for crystallization) shows the most acceptable model.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.21Ang From Br3   -2.20 eA-3

Author Response: This might be caused by wrongly assigned atom types and other model errors. But It was also confirmed from (1H)NMR and HRMS that our crystal structure is correct.It has been tried with various models considering different type of solvent molecules. But DMSO (which was used as solvent for crystallization) shows the most acceptable model.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.77Ang From Br1   -1.96 eA-3

Author Response: This might be caused by wrongly assigned atom types and other model errors. But It was also confirmed from (1H)NMR and HRMS that our crystal structure is correct.It has been tried with various models considering different type of solvent molecules. But DMSO (which was used as solvent for crystallization) shows the most acceptable model.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.74Ang From Br2 -1.95 eA-3

Author Response: This might be caused by wrongly assigned atom types and other model errors. But It was also confirmed from (1H)NMR and HRMS that our crystal structure is correct.It has been tried with various models considering different type of solvent molecules. But DMSO (which was used as solvent for crystallization) shows the most acceptable model.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.77Ang From Br3 -1.89 eA-3

Author Response: This might be caused by wrongly assigned atom types and other model errors. But It was also confirmed from (1H)NMR and HRMS that our crystal structure is correct.It has been tried with various models considering different type of solvent molecules. But DMSO (which was used as solvent for crystallization) shows the most acceptable model.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.73Ang From Br3 -1.89 eA-3

Author Response: This might be caused by wrongly assigned atom types and other model errors. But It was also confirmed from (1H)NMR and HRMS that our crystal structure is correct.It has been tried with various models considering different type of solvent molecules. But DMSO (which was used as solvent for crystallization) shows the most acceptable model.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.81Ang From Br4 -1.78 eA-3

Author Response: This might be caused by wrongly assigned atom types and other model errors. But It was also confirmed from (1H)NMR and HRMS that our crystal structure is correct.It has been tried with various models considering different type of solvent molecules. But DMSO (which was used as solvent for crystallization) shows the most acceptable model.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.65Ang From Ni1 -1.73 eA-3

Author Response: This might be caused by wrongly assigned atom types and other model errors. But It was also confirmed from (1H)NMR and HRMS that our crystal structure is correct.It has been tried with various models considering different type of solvent molecules. But DMSO (which was used as solvent for crystallization) shows the most acceptable model.

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.37Ang From C37           -1.72 eA-3
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Author Response: This might be caused by wrongly assigned atom types and other model errors. But It was also confirmed from (1H)NMR and HRMS that our crystal structure is correct.It has been tried with various models considering different type of solvent molecules. But DMSO (which was used as solvent for crystallization) shows the most acceptable model.

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.78Ang From Br2           -1.65 eA-3
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Author Response: This might be caused by wrongly assigned atom types and other model errors. But It was also confirmed from (1H)NMR and HRMS that our crystal structure is correct.It has been tried with various models considering different type of solvent molecules. But DMSO (which was used as solvent for crystallization) shows the most acceptable model.

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.29Ang From Br1           -1.56 eA-3
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Author Response: This might be caused by wrongly assigned atom types and other model errors. But It was also confirmed from (1H)NMR and HRMS that our crystal structure is correct.It has been tried with various models considering different type of solvent molecules. But DMSO (which was used as solvent for crystallization) shows the most acceptable model.

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PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.00Ang From N2      .       1.46 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3B       .      -0.45 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H5B       .      -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6B       .      -0.45 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H8A       .      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H20B      .      -0.68 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H21A      .      -0.51 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H21B      .      -0.42 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H36B      .      -0.52 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H37C      .      -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H40A      .      -0.51 eA-3
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Alert level G

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PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Br3      ..Br4      .       3.60 Ang.
                                          3/2-x,1/2+y,z  =      6_765 Check
PLAT480_ALERT_4_G Long H...A H-Bond Reported H40C     ..BR3      .       3.06 Ang.
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PLAT480_ALERT_4_G Long H...A H-Bond Reported H40B     ..BR1      .       3.11 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H40A     ..BR2      .       2.98 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H36B     ..O33      .       2.62 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H28      ..BR2      .       3.02 Ang.
PLAT793_ALERT_4_G Model has Chirality at C7          (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C23         (Centro SPGR)          S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1       (II)      .       2.09 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        155 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  8 ALERT level B = A potentially serious problem, consider carefully
 42 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 14 ALERT level G = General information/check it is not something unexpected

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

PLATON version of 12/09/2022; check.def file version of 09/08/2022

Datablock T7_0ma - ellipsoid plot